Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2014

- Supplementary Information-

A DFT-based model for calculating solvolytic reactivity. Nucleofugality of aliphatic carboxylates in terms of N_f parameters

Bernard Denegri,* Mirela Matić and Olga Kronja

University of Zagreb, Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, 10000 Zagreb, Croatia

Table of contents

I. Tables……..……..*S2*

Table S1. Calculated solvolytic reactivities for the reference dianisylmethyl carboxylates and corresponding calculated nucleofugalities of carboxylate leaving groups……...*S3*

Table S2. Calculated solvolytic reactivities for other dianisylmethyl carboxylates and corresponding calculated nucleofugalities of carboxylate leaving groups ……..…...*S6*

Table S3. Activation energies for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated with different theoretical methods by using IEFPCM …..……....*S13*

Table S4. Selected geometrical parameters of *cis*-2,3-dihydroxycyclopropyl carboxylate structures optimized at the M06-2X/AUG-cc-pVTZ level of theory by using IEFPCM solvation model ……...…...*S21*

II. Correlations …….....……..……....*S24*

II.1. Correlations of experimental free energies of activation for solvolyses of dianisylmethyl carboxylates in 80% ethanol against calculated free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates…….……..….*S25*

II.2. Correlations of experimental free energies of activation for solvolyses of dianisylmethyl carboxylates in aqueous ethanol mixtures against free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the M06-2X/AUG-cc-pVTZ level of theory in the presence of IEFPCM solvation model ……..*S31*

III. Geometries of *cis*-2,3-dihydroxycyclopropyl carboxylates and geometries of related heterolytic transition states optimized at the IEFPCM-M06-2X/AUG-cc-pVTZ level *S33*

IV. Coordinates and energies…….…….….*S42*

V. Literature experimental data……..…….…….....*S118*

VI. References……..….*S121*

I.

Tables

Table S1. Calculated solvolytic reactivities for the reference dianisylmethyl carboxylates and corresponding calculated nucleofugalities of carboxylate leaving groups

Solvent [a]	**Carboxylate**	$\Delta G^{\ddagger}$**calc** [b]	**log** k**calc** [c]	s_f**estim** [d,f]	N_f**calc** [e,f]
90E10W	Formate	21.30 (+0.36)	−2.82 (−0.26)	1.07 (+0.01)	−2.64 (−0.23)
	Acetate	23.50 (+0.10)	−4.43 (−0.07)	1.15 [g]	−3.85 (−0.06)
	2-Methylpropanoate	23.80 (−0.29)	−4.65 (+0.22)	1.17 [g]	−3.98 (+0.18)
	2,2-Dimethylpropanoate	24.38 (−0.34)	−5.08 (+0.25)	1.20 [g]	−4.23 (+0.21)
	Fluoroacetate	20.46 (+0.27)	−2.20 (−0.19)	1.04 (±0.00)	−2.12 (−0.18)
	Chloroacetate	20.06 (−0.49)	−1.91 (+0.36)	1.03 (+0.02)	−1.86 (+0.41)
	Bromoacetate	20.28 (−0.31)	−2.07 (+0.23)	1.03 (−0.02)	−2.01 (+0.15)
	Dichloroacetate	18.35 (−0.15)	−0.66 (+0.11)	0.96 (−0.01)	−0.68 (+0.11)
	Trifluoroacetate	15.86 (−0.19)	1.17 (+0.14)	0.87 (+0.01)	1.34 (+0.15)
	Trichloroacetate	16.42 (±0.00)	0.76 (±0.00)	0.89 (−0.01)	0.85 (+0.01)
	Heptafluorobutanoate	15.73 (−0.08)	1.26 (+0.05)	0.87 (−0.01)	1.45 (+0.08)
80E20W	Formate	21.06 (+0.59)	−2.64 (−0.43)	1.05 (+0.01)	−2.52 (−0.39)
	Acetate	23.26 (+0.29)	−4.26 (−0.22)	1.12 [g]	−3.80 (−0.19)
	2-Methylpropanoate	23.56 (−0.12)	−4.48 (+0.08)	1.15 [g]	−3.89 (+0.08)
	2,2-Dimethylpropanoate	24.14 (−0.17)	−4.90 (+0.12)	1.17 [g]	−4.19 (+0.10)
	Fluoroacetate	20.22 (+0.43)	−2.03 (−0.32)	1.02 (+0.02)	−1.99 (−0.27)
	Chloroacetate	19.82 (−0.33)	−1.73 (+0.24)	1.01 (±0.00)	−1.72 (+0.23)
	Bromoacetate	20.04 (−0.10)	−1.90 (+0.07)	1.01 (−0.01)	−1.88 (+0.05)
	Dichloroacetate	18.11 (−0.08)	−0.48 (+0.06)	0.94 (+0.03)	−0.51 (+0.08)

Solvent [a]	**Carboxylate**	$\Delta G^{\ddagger}$**calc** [b]	**log** k**calc** [c]	s_f**estim** [d,f]	N_f**calc** [e,f]
	Trifluoroacetate	15.62 (−0.24)	1.34 (+0.18)	0.85 (+0.03)	1.58 (+0.16)
	Trichloroacetate	16.18 (+0.21)	0.93 (−0.16)	0.87 (−0.03)	1.07 (−0.14)
	Heptafluorobutanoate	15.49 (+0.20)	1.44 (−0.14)	0.85 (−0.03)	1.69 (−0.11)
70E30W	Formate	20.76 (+0.63)	−2.42 (−0.46)	1.01 (±0.00)	−2.40 (−0.44)
	Acetate	22.99 (+0.32)	−4.06 (−0.24)	1.06 [g]	−3.83 (−0.23)
	2-Methylpropanoate	23.29 (−0.27)	−4.28 (+0.20)	1.09 [g]	−3.93 (+0.18)
	2,2-Dimethylpropanoate	23.88 (−0.22)	−4.71 (+0.16)	1.10 [g]	−4.28 (+0.15)
	Fluoroacetate	19.92 (+0.40)	−1.81 (−0.29)	0.98 (+0.02)	−1.85 (−0.26)
	Chloroacetate	19.51 (−0.38)	−1.51 (+0.28)	0.97 (±0.00)	−1.55 (+0.29)
	Bromoacetate	19.73 (−0.16)	−1.67 (+0.11)	0.98 (±0.00)	−1.70 (+0.13)
	Dichloroacetate	17.78 (−0.13)	−0.24 (+0.09)	0.92 (+0.02)	−0.26 (+0.11)
	Trifluoroacetate	15.27 (−0.09)	1.60 (+0.06)	0.85 (+0.01)	1.88 (+0.05)
	Trichloroacetate	15.83 (+0.15)	1.19 (−0.11)	0.86 (−0.03)	1.38 (−0.08)
	Heptafluorobutanoate	15.13 (+0.01)	1.70 (−0.01)	0.84 (−0.02)	2.03 (+0.04)
60E40W	Formate	20.36 (+0.51)	−2.13 (−0.37)	0.95 (±0.00)	−2.24 (−0.37)
	Acetate	22.59 (+0.18)	−3.77 (−0.14)	1.00 [g]	−3.77 (−0.14)
	2-Methylpropanoate	22.89 (−0.48)	−3.99 (+0.35)	1.02 [g]	−3.91 (+0.34)
	2,2-Dimethylpropanoate	23.48 (−0.36)	−4.42 (+0.26)	1.03 [g]	−4.29 (+0.25)
	Fluoroacetate	19.52 (+0.27)	−1.51 (−0.19)	0.94 (+0.02)	−1.61 (−0.14)
	Chloroacetate	19.11 (−0.54)	−1.21 (+0.40)	0.93 (±0.00)	−1.31 (+0.44)
	Bromoacetate	19.33 (−0.31)	−1.38 (+0.22)	0.93 (−0.01)	−1.48 (+0.24)

Solvent [a]	**Carboxylate**	$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d,f]	N_f^{calc} [e,f]
	Dichloroacetate	17.38 (−0.35)	0.05 (+0.25)	0.89 (+0.04)	0.06 (+0.30)
	Trifluoroacetate	14.87 (−0.22)	1.89 (+0.16)	0.83 (+0.01)	2.28 (+0.17)
	Trichloroacetate	15.43 (−0.01)	1.48 (±0.00)	0.85 (−0.02)	1.74 (+0.04)
	Heptafluorobutanoate	14.73 (−0.02)	2.00 (+0.02)	0.83 (−0.03)	2.40 (+0.10)

[a] Binary solvents are v/v at 25 °C. E = ethanol, W = water. [b] in kcal mol^{-1}. Obtained from $\Delta G^{\ddagger}$ (dianisylmethyl carboxylates) versus $\Delta G^{\ddagger model}$ (M06-2X/AUG-cc-pVTZ level) plots given in Tables 1 and 2. Deviations from experimental values ($\Delta G^{\ddagger calc} - \Delta G^{\ddagger}$) are given in parentheses. [c] Logarithms of solvolytic first-order rate constants at 25 °C obtained from $\Delta G^{\ddagger calc}$. Deviations from experimental values (log k^{calc} − log k) are given in parentheses. [d] s_f parameters estimated from the correlation of s_f versus log k (25 °C) for solvolysis of dianisylmethyl carboxylates in an appropriate solvent. The correlation plots are presented in reference 1a. Deviations from experimental s_f values ($s_f^{estim} - s_f$) are given in parentheses. [e] Calculated from the log k^{calc} and appropriate s_f^{estim} by using equation (1). E_f value for the dianisylmethyl electrofuge is 0.00. Deviations from experimental values ($N_f^{calc} - N_f$) are given in parentheses. [f] Experimental data are given in reference 1. [g] s_f parameters were previously obtained from the s_f versus log k (25 °C) correlation plots and presented in reference 1a.

Table S2. Calculated solvolytic reactivities for other dianisylmethyl carboxylates and corresponding calculated nucleofugalities of carboxylate leaving groups

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger}$**calc** [b]	**log** k**calc** [c]	s_f**estim** [d]	N_f**calc** [e]
90E10W	Propionate (Propanoate)	$C_2H_5CO_2^-$	23.24	−4.24	1.14	−3.72
	Butanoate (Butyrate)	$C_3H_7CO_2^-$	23.65	−4.54	1.16	−3.92
	Phenylacetate	$C_6H_5CH_2CO_2^-$	22.52	−3.71	1.12	−3.32
	Propenoate (Acrylate)	$CH_2{=}CHCO_2^-$	22.32	−3.57	1.11	−3.21
	Propynoate (Propiolate)	$CH{\equiv}CCO_2^-$	19.21	−1.29	0.99	−1.30
	Difluoroacetate	$CHF_2CO_2^-$	17.95	−0.36	0.95	−0.38
	Dibromoacetate	$CHBr_2CO_2^-$	17.74	−0.21	0.94	−0.22
	Tribromoacetate	$CBr_3CO_2^-$	16.71	0.54	0.90	0.61
	Pentafluoropropanoate	$C_2F_5CO_2^-$	15.75	1.25	0.87	1.44
	Pentachloropropanoate	$C_2Cl_5CO_2^-$	16.68	0.57	0.90	0.63
	Pentabromopropanoate	$C_2Br_5CO_2^-$	16.95	0.37	0.91	0.41
	Heptachlorobutanoate	$C_3Cl_7CO_2^-$	16.69	0.56	0.90	0.62
	3,3,3-Trifluoropropanoate	$CF_3CH_2CO_2^-$	20.03	−1.89	1.02	−1.85
	Hexafluoroisobutanoate	$(CF_3)_2CHCO_2^-$	18.42	−0.71	0.97	−0.73
	Nonafluorotrimethylacetate	$(CF_3)_3CCO_2^-$	15.16	1.68	0.85	1.98
	Cyanoacetate	$NCCH_2CO_2^-$	19.24	−1.31	1.00	−1.31
	Dicyanoacetate	$(NC)_2CHCO_2^-$	15.32	1.56	0.85	1.84
	Tricyanoacetate	$(NC)_3CCO_2^-$	11.76	4.17	0.72	5.80
	Nitroacetate	$O_2NCH_2CO_2^-$	18.04	−0.43	0.95	−0.45

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	Dinitroacetate	$(O_2N)_2CHCO_2^-$	14.29	2.32	0.81	2.86
	Trinitroacetate	$(O_2N)_3CCO_2^-$	10.85	4.84	0.69	7.01
	2-Cyanopropenoate (Cyanoacrylate)	$CH_2=C(CN)CO_2^-$	18.87	−1.04	0.98	−1.06
	2-Hydroxyethanoate (Glycolate)	$HOCH_2CO_2^-$	20.74	−2.41	1.05	−2.29
	2-Hydroxypropanoate (Lactate)	$CH_3(HO)CHCO_2^-$	21.08	−2.66	1.06	−2.51
	2,3-Dihydroxypropanoate (Glycerate)	$HOCH_2(HO)CHCO_2^-$	20.49	−2.23	1.04	−2.14
	Oxoethanoate (Glyoxylate)	$OHCCO_2^-$	18.05	−0.44	0.95	−0.46
	2-Oxopropanoate (Pyruvate)	$CH_3C(O)CO_2^-$	19.68	−1.63	1.01	−1.62
	3-Oxopropanoate (Formylacetate)	$OHCCH_2CO_2^-$	22.42	−3.64	1.11	−3.28
	2-Oxobutanoate (α-Ketobutyrate)	$CH_3CH_2C(O)CO_2^-$	20.00	−1.87	1.02	−1.83
	3-Oxobutanoate (Acetoacetate)	$H_3CC(O)CH_2CO_2^-$	22.35	−3.59	1.11	−3.23
	Oxalate, 1. dissociation	$RO_2CCCO_2^-$	18.55	−0.80	0.97	−0.83
	Oxalate, 2. dissociation	$^-O_2CCCO_2^-$	23.61	−4.51	1.16	−3.89
	Malonate, 1. dissociation	$RO_2CCH_2CO_2^-$	21.77	−3.16	1.09	−2.90
	Malonate, 2. dissociation	$^-O_2CCH_2CO_2^-$	25.15	−5.64	1.21	−4.66
80E20W	Propionate (Propanoate)	$C_2H_5CO_2^-$	23.00	−4.07	1.12	−3.63
	Butanoate (Butyrate)	$C_3H_7CO_2^-$	23.41	−4.37	1.14	−3.83
	Phenylacetate	$C_6H_5CH_2CO_2^-$	22.28	−3.54	1.10	−3.22
	Propenoate (Acrylate)	$CH_2=CHCO_2^-$	22.08	−3.39	1.09	−3.11
	Propynoate (Propiolate)	$CH\equiv CCO_2^-$	18.97	−1.11	0.98	−1.13
	Difluoroacetate	$CHF_2CO_2^-$	17.71	−0.19	0.93	−0.20

Solvent [a]	Carboxylate		$\Delta G^{\ddagger calc}$ [b]	log k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	Dibromoacetate	$CHBr_2CO_2^-$	17.50	−0.03	0.92	−0.04
	Tribromoacetate	$CBr_3CO_2^-$	16.47	0.72	0.88	0.82
	Pentafluoropropanoate	$C_2F_5CO_2^-$	15.51	1.42	0.85	1.68
	Pentachloropropanoate	$C_2Cl_5CO_2^-$	16.44	0.74	0.88	0.84
	Pentabromopropanoate	$C_2Br_5CO_2^-$	16.71	0.54	0.89	0.61
	Heptachlorobutanoate	$C_3Cl_7CO_2^-$	16.45	0.74	0.88	0.84
	3,3,3-Trifluoropropanoate	$CF_3CH_2CO_2^-$	19.79	−1.71	1.01	−1.70
	Hexafluoroisobutanoate	$(CF_3)_2CHCO_2^-$	18.18	−0.53	0.95	−0.56
	Nonafluorotrimethylacetate	$(CF_3)_3CCO_2^-$	14.92	1.86	0.83	2.24
	Cyanoacetate	$NCCH_2CO_2^-$	19.00	−1.13	0.98	−1.16
	Dicyanoacetate	$(NC)_2CHCO_2^-$	15.08	1.74	0.83	2.10
	Tricyanoacetate	$(NC)_3CCO_2^-$	11.52	4.35	0.70	6.21
	Nitroacetate	$O_2NCH_2CO_2^-$	17.80	−0.25	0.93	−0.27
	Dinitroacetate	$(O_2N)_2CHCO_2^-$	14.05	2.49	0.80	3.12
	Trinitroacetate	$(O_2N)_3CCO_2^-$	10.61	5.02	0.67	7.49
	2-Cyanopropenoate (Cyanoacrylate)	$CH_2=C(CN)CO_2^-$	18.63	−0.86	0.96	−0.90
	2-Hydroxyethanoate (Glycolate)	$HOCH_2CO_2^-$	20.50	−2.23	1.03	−2.17
	2-Hydroxypropanoate (Lactate)	$CH_3(HO)CHCO_2^-$	20.84	−2.48	1.04	−2.39
	2,3-Dihydroxypropanoate (Glycerate)	$HOCH_2(HO)CHCO_2^-$	20.25	−2.05	1.02	−2.01
	Oxoethanoate (Glyoxylate)	$OHCCO_2^-$	17.81	−0.26	0.93	−0.28
	2-Oxopropanoate (Pyruvate)	$CH_3C(O)CO_2^-$	19.44	−1.46	0.99	−1.47

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	3-Oxopropanoate (Formylacetate)	$OHCCH_2CO_2^-$	22.18	−3.46	1.09	−3.18
	2-Oxobutanoate (α-Ketobutyrate)	$CH_3CH_2C(O)CO_2^-$	19.76	−1.69	1.00	−1.69
	3-Oxobutanoate (Acetoacetate)	$H_3CC(O)CH_2CO_2^-$	22.11	−3.41	1.09	−3.13
	Oxalate, 1. dissociation	$RO_2CCO_2^-$	18.31	−0.63	0.95	−0.66
	Oxalate, 2. dissociation	$^-O_2CCO_2^-$	23.37	−4.34	1.14	−3.80
	Malonate, 1. dissociation	$RO_2CCH_2CO_2^-$	21.53	−2.99	1.07	−2.79
	Malonate, 2. dissociation	$^-O_2CCH_2CO_2^-$	24.91	−5.47	1.19	−4.59
70E30W	Propionate (Propanoate)	$C_2H_5CO_2^-$	22.73	−3.87	1.06	−3.65
	Butanoate (Butyrate)	$C_3H_7CO_2^-$	23.14	−4.17	1.08	−3.86
	Phenylacetate	$C_6H_5CH_2CO_2^-$	22.00	−3.33	1.04	−3.20
	Propenoate (Acrylate)	$CH_2=CHCO_2^-$	21.80	−3.19	1.04	−3.06
	Propynoate (Propiolate)	$CH\equiv CCO_2^-$	18.65	−0.88	0.95	−0.92
	Difluoroacetate	$CHF_2CO_2^-$	17.38	0.05	0.91	0.06
	Dibromoacetate	$CHBr_2CO_2^-$	17.16	0.21	0.90	0.24
	Tribromoacetate	$CBr_3CO_2^-$	16.12	0.98	0.87	1.12
	Pentafluoropropanoate	$C_2F_5CO_2^-$	15.15	1.69	0.84	2.01
	Pentachloropropanoate	$C_2Cl_5CO_2^-$	16.09	1.00	0.87	1.15
	Pentabromopropanoate	$C_2Br_5CO_2^-$	16.36	0.80	0.88	0.91
	Heptachlorobutanoate	$C_3Cl_7CO_2^-$	16.10	0.99	0.87	1.14
	3,3,3-Trifluoropropanoate	$CF_3CH_2CO_2^-$	19.48	−1.49	0.97	−1.53
	Hexafluoroisobutanoate	$(CF_3)_2CHCO_2^-$	17.85	−0.29	0.92	−0.32

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	Nonafluorotrimethylacetate	$(CF_3)_3CCO_2^-$	14.55	2.13	0.82	2.60
	Cyanoacetate	$NCCH_2CO_2^-$	18.68	−0.90	0.95	−0.95
	Dicyanoacetate	$(NC)_2CHCO_2^-$	14.72	2.00	0.83	2.41
	Tricyanoacetate	$(NC)_3CCO_2^-$	11.12	4.64	0.72	6.45
	Nitroacetate	$O_2NCH_2CO_2^-$	17.46	0.00	0.91	−0.01
	Dinitroacetate	$(O_2N)_2CHCO_2^-$	13.67	2.77	0.80	3.47
	Trinitroacetate	$(O_2N)_3CCO_2^-$	10.20	5.32	0.70	7.60
	2-Cyanopropenoate (Cyanoacrylate)	$CH_2=C(CN)CO_2^-$	18.31	−0.63	0.94	−0.67
	2-Hydroxyethanoate (Glycolate)	$HOCH_2CO_2^-$	20.20	−2.01	0.99	−2.03
	2-Hydroxypropanoate (Lactate)	$CH_3(HO)CHCO_2^-$	20.54	−2.26	1.00	−2.26
	2,3-Dihydroxypropanoate (Glycerate)	$HOCH_2(HO)CHCO_2^-$	19.95	−1.83	0.98	−1.87
	Oxoethanoate (Glyoxylate)	$OHCCO_2^-$	17.48	−0.02	0.91	−0.02
	2-Oxopropanoate (Pyruvate)	$CH_3C(O)CO_2^-$	19.13	−1.23	0.96	−1.28
	3-Oxopropanoate (Formylacetate)	$OHCCH_2CO_2^-$	21.90	−3.26	1.04	−3.13
	2-Oxobutanoate (α-Ketobutyrate)	$CH_3CH_2C(O)CO_2^-$	19.45	−1.46	0.97	−1.51
	3-Oxobutanoate (Acetoacetate)	$H_3CC(O)CH_2CO_2^-$	21.83	−3.21	1.04	−3.08
	Oxalate, 1. dissociation	$RO_2CCCO_2^-$	17.98	−0.39	0.93	−0.42
	Oxalate, 2. dissociation	$^-O_2CCCO_2^-$	23.10	−4.14	1.08	−3.83
	Malonate, 1. dissociation	$RO_2CCH_2CO_2^-$	21.24	−2.78	1.02	−2.72
	Malonate, 2. dissociation	$^-O_2CCH_2CO_2^-$	24.65	−5.28	1.12	−4.71
60E40W	Propionate (Propanoate)	$C_2H_5CO_2^-$	22.33	−3.57	1.00	−3.57

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	Butanoate (Butyrate)	$C_3H_7CO_2^-$	22.74	−3.88	1.01	−3.84
	Phenylacetate	$C_6H_5CH_2CO_2^-$	21.60	−3.04	0.98	−3.10
	Propenoate (Acrylate)	$CH_2{=}CHCO_2^-$	21.40	−2.89	0.98	−2.95
	Propynoate (Propiolate)	$CH{\equiv}CCO_2^-$	18.25	−0.58	0.91	−0.64
	Difluoroacetate	$CHF_2CO_2^-$	16.98	0.35	0.88	0.39
	Dibromoacetate	$CHBr_2CO_2^-$	16.76	0.51	0.87	0.58
	Tribromoacetate	$CBr_3CO_2^-$	15.72	1.27	0.85	1.49
	Pentafluoropropanoate	$C_2F_5CO_2^-$	14.75	1.98	0.83	2.39
	Pentachloropropanoate	$C_2Cl_5CO_2^-$	15.69	1.29	0.85	1.52
	Pentabromopropanoate	$C_2Br_5CO_2^-$	15.96	1.09	0.86	1.27
	Heptachlorobutanoate	$C_3Cl_7CO_2^-$	15.70	1.29	0.85	1.51
	3,3,3-Trifluoropropanoate	$CF_3CH_2CO_2^-$	19.08	−1.19	0.93	−1.28
	Hexafluoroisobutanoate	$(CF_3)_2CHCO_2^-$	17.45	0.00	0.89	0.00
	Nonafluorotrimethylacetate	$(CF_3)_3CCO_2^-$	14.15	2.42	0.82	2.95
	Cyanoacetate	$NCCH_2CO_2^-$	18.28	−0.61	0.91	−0.67
	Dicyanoacetate	$(NC)_2CHCO_2^-$	14.32	2.30	0.82	2.79
	Tricyanoacetate	$(NC)_3CCO_2^-$	10.72	4.94	0.74	6.67
	Nitroacetate	$O_2NCH_2CO_2^-$	17.06	0.29	0.88	0.33
	Dinitroacetate	$(O_2N)_2CHCO_2^-$	13.27	3.07	0.80	3.83
	Trinitroacetate	$(O_2N)_3CCO_2^-$	9.80	5.61	0.72	7.79
	2-Cyanopropenoate (Cyanoacrylate)	$CH_2{=}C(CN)CO_2^-$	17.91	−0.33	0.90	−0.37

Solvent [a]	**Carboxylate**		$\Delta G^{\ddagger calc}$ [b]	**log** k^{calc} [c]	s_f^{estim} [d]	N_f^{calc} [e]
	2-Hydroxyethanoate (Glycolate)	$HOCH_2CO_2^-$	19.80	−1.72	0.94	−1.83
	2-Hydroxypropanoate (Lactate)	$CH_3(HO)CHCO_2^-$	20.14	−1.97	0.95	−2.07
	2,3-Dihydroxypropanoate (Glycerate)	$HOCH_2(HO)CHCO_2^-$	19.55	−1.54	0.94	−1.64
	Oxoethanoate (Glyoxylate)	$OHCCO_2^-$	17.08	0.27	0.88	0.31
	2-Oxopropanoate (Pyruvate)	$CH_3C(O)CO_2^-$	18.73	−0.93	0.92	−1.01
	3-Oxopropanoate (Formylacetate)	$OHCCH_2CO_2^-$	21.50	−2.97	0.98	−3.03
	2-Oxobutanoate (α-Ketobutyrate)	$CH_3CH_2C(O)CO_2^-$	19.05	−1.17	0.93	−1.26
	3-Oxobutanoate (Acetoacetate)	$H_3CC(O)CH_2CO_2^-$	21.43	−2.91	0.98	−2.97
	Oxalate, 1. dissociation	$RO_2CCCO_2^-$	17.58	−0.09	0.89	−0.10
	Oxalate, 2. dissociation	$^-O_2CCCO_2^-$	22.70	−3.85	1.01	−3.81
	Malonate, 1. dissociation	$RO_2CCH_2CO_2^-$	20.84	−2.48	0.96	−2.59
	Malonate, 2. dissociation	$^-O_2CCH_2CO_2^-$	24.25	−4.98	1.04	−4.79

[a] Binary solvents are v/v at 25 °C. E = ethanol, W = water. [b] in kcal mol^{-1}. Obtained from the correlations of experimental solvolysis $\Delta G^{\ddagger}$ (25 °C) for dianisylmethyl carboxylates versus heterolytic $\Delta G^{\ddagger}$ (25 °C) for *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the IEFPCM-M06-2X/AUG-cc-pVTZ level of theory. [c] Logarithms of solvolytic first-order rate constants at 25 °C obtained from $\Delta G^{\ddagger calc}$. [d] s_f values estimated from the correlation of s_f versus log k (25 °C) for solvolysis of dianisylmethyl carboxylates in an appropriate solvent. The correlation plots are presented in reference 1a. [e] Calculated from k^{calc} and appropriate s_f^{estim} by using the equation $\log k = s_f (E_f + N_f)$. E_f value for the dianisylmethyl electrofuge is 0.00.

Table S3. Activation energies (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated with different theoretical methods

Method	**Solvation model**	**Basis Set**	**Carboxylate**	$\Delta E^{\ddagger \mathbf{model}}$ [*a*]	$\Delta H^{\ddagger \mathbf{model}}$ [*b*]	$\Delta G^{\ddagger \mathbf{model}}$ [*c*]
M06-2X	IEFPCM	AUG-cc-pVTZ	***Reference Carboxylates***			
			Formate	32.04	32.24	31.36
			Acetate	34.55	34.62	33.83
			2-Methylpropanoate (Isobutyrate)	34.87	34.89	34.17
			2,2-Dimethylpropanoate (Pivalate)	35.05	34.97	34.82
			Fluoroacetate	31.08	31.09	30.42
			Chloroacetate	30.87	30.92	29.97
			Bromoacetate	30.77	30.82	30.21
			Dichloroacetate	28.48	28.51	28.04
			Trifluoroacetate	25.99	26.01	25.25
			Trichloroacetate	26.40	26.46	25.88
			Heptafluorobutanoate	24.91	24.87	25.10
			Other Carboxylates			
			Propanoate (Propionate)	34.88	34.97	33.54
			Butanoate (Butyrate)	34.87	34.92	34.00
			Phenylacetate	33.70	33.72	32.73
			Propenoate (Acrylate)	33.70	33.84	32.51
			Propynoate (Propiolate)	29.66	29.68	29.01
			Difluoroacetate	28.37	28.41	27.60
			Dibromoacetate	28.49	28.55	27.36
			Tribromoacetate	26.67	26.65	26.19
			Pentafluoropropanoate	25.60	25.59	25.12

Method	Solvation model	Basis Set	Carboxylate	$\Delta E^{\ddagger model}$ [a]	$\Delta H^{\ddagger model}$ [b]	$\Delta G^{\ddagger model}$ [c]
			Pentachloropropanoate	26.89	26.89	26.17
			Pentabromopropanoate	27.22	27.27	26.47
			Heptachlorobutanoate	26.63	26.67	26.18
			3,3,3-Trifluoropropanoate	31.06	31.13	29.93
			Hexafluoroisobutanoate	27.98	27.94	28.12
			Nonafluorotrimethylacetate	24.93	24.95	24.46
			Cyanoacetate	29.77	29.85	29.04
			Dicyanoacetate	25.23	25.29	24.64
			Tricyanoacetate	20.96	21.02	20.64
			Nitroacetate	28.09	28.09	27.69
			Dinitroacetate	24.28	24.36	23.48
			Trinitroacetate	20.51	20.57	19.62
			2-Cyanopropenoate (Cyanoacrylate)	29.61	29.71	28.63
			2-Hydroxyethanoate (Glycolate)	31.11	30.97	30.73
			2-Hydroxypropanoate (Lactate)	31.28	31.13	31.11
			2,3-Dihydroxypropanoate (Glycerate)	31.07	30.97	30.45
			Oxoethanoate (Glyoxylate)	28.78	28.87	27.71
			2-Oxopropanoate (Pyruvate)	30.18	30.11	29.54
			3-Oxopropanoate (Formylacetate)	32.89	32.85	32.62
			2-Oxobutanoate (α-Ketobutyrate)	30.32	30.26	29.90
			3-Oxobutanoate (Acetoacetate)	33.31	33.35	32.54
			Oxalate, 1. dissociation	29.03	28.99	28.27
			Oxalate, 2. dissociation	34.62	34.72	33.95
			Malonate, 1. dissociation	32.48	32.47	31.89

Method	Solvation model	Basis Set	Carboxylate	$\Delta E^{\ddagger \text{model}}$ [a]	$\Delta H^{\ddagger \text{model}}$ [b]	$\Delta G^{\ddagger \text{model}}$ [c]
			Malonate, 2. dissociation	36.58	36.63	35.68
M06-2X	IEFPCM	AUG-cc-pVDZ	***Reference Carboxylates***			
			Formate	32.83	32.98	32.27
			Acetate	35.29	35.36	34.40
			2-Methylpropanoate (Isobutyrate)	35.66	35.67	34.75
			2,2-Dimethylpropanoate (Pivalate)	35.87	35.75	35.83
			Fluoroacetate	31.77	31.80	30.78
			Chloroacetate	31.47	31.49	30.67
			Bromoacetate	31.29	31.33	30.69
			Dichloroacetate	28.89	28.92	28.35
			Trifluoroacetate	26.70	26.66	26.37
			Trichloroacetate	–	–	–
			Heptafluorobutanoate	25.91	25.81	26.32
M06-2X	IEFPCM	6-311+G(3df,2p)	***Reference Carboxylates***			
			Formate	32.85	33.04	32.18
			Acetate	35.32	35.41	34.54
			2-Methylpropanoate (Isobutyrate)	35.67	35.72	34.63
			2,2-Dimethylpropanoate (Pivalate)	35.86	35.79	35.54
			Fluoroacetate	31.90	31.93	31.17
			Chloroacetate	31.68	31.70	30.87
			Bromoacetate	31.51	31.54	30.96
			Dichloroacetate	29.08	29.14	28.42
			Trifluoroacetate	26.89	26.86	26.49
			Trichloroacetate	27.12	27.17	26.70

Method	**Solvation model**	**Basis Set**	**Carboxylate**	$\Delta E^{\ddagger \text{model}}$ [*a*]	$\Delta H^{\ddagger \text{model}}$ [*b*]	$\Delta G^{\ddagger \text{model}}$ [*c*]
			Heptafluorobutanoate	26.00	25.94	26.31
M06-2X	IEFPCM	6-31+G(d)	***Reference Carboxylates***			
			Formate	33.67	33.95	32.87
			Acetate	36.31	36.42	35.56
			Isobutanoate	36.79	36.78	36.28
			Trimethylacetate	36.83	36.83	36.44
			Fluoroacetate	32.61	32.70	31.80
			Chloroacetate	32.31	32.45	31.26
			Bromoacetate	32.44	32.57	31.63
			Dichloroacetate	29.70	29.76	29.17
			Trifluoroacetate	27.40	27.41	27.12
			Trichloroacetate	27.54	27.67	26.52
			Heptafluorobutanoate	26.48	26.51	26.41
B3LYP	IEFPCM	AUG-cc-pVTZ	*Reference*			
			Formate	20.85	20.96	19.80
			Acetate	–	–	–
			Isobutanoate	23.22	23.19	22.12
			Trimethylacetate	23.31	23.31	22.51
			Fluoroacetate	20.15	20.15	19.42
			Chloroacetate	–	–	–
			Bromoacetate	–	–	–
			Dichloroacetate	18.28	18.29	18.34
			Trifluoroacetate	16.46	16.48	15.69
			Trichloroacetate	16.77	16.75	15.86

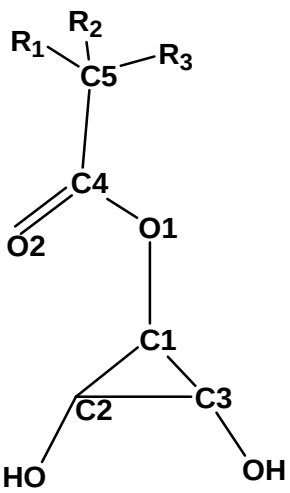
Method	Solvation model	Basis Set	Carboxylate	$\Delta E^{\ddagger \text{model}}$ [a]	$\Delta H^{\ddagger \text{model}}$ [b]	$\Delta G^{\ddagger \text{model}}$ [c]
			Heptafluorobutanoate	16.20	16.19	15.89
B3LYP	IEFPCM	6-311+G(3df,2p)	***Reference Carboxylates***			
			Formate	21.23	21.33	20.30
			Acetate	–	–	–
			2-Methylpropanoate (Isobutyrate)	23.56	23.52	22.68
			2,2-Dimethylpropanoate (Pivalate)	23.65	23.65	22.92
			Fluoroacetate	20.51	20.51	19.78
			Chloroacetate	–	–	–
			Bromoacetate	20.15	20.21	19.07
			Dichloroacetate	18.65	18.66	18.10
			Trifluoroacetate	16.81	16.83	16.10
			Trichloroacetate	17.13	17.11	16.23
			Heptafluorobutanoate	16.55	16.54	16.21
mPW3PBE	IEFPCM	6-311+G(3df,2p)	***Reference Carboxylates***			
			Formate	24.45	24.58	23.34
			Acetate	26.81	26.82	25.83
			2-Methylpropanoate (Isobutyrate)	27.04	27.02	26.72
			2,2-Dimethylpropanoate (Pivalate)	27.01	27.05	25.74
			Fluoroacetate	–	–	–
			Chloroacetate	–	–	–
			Bromoacetate	–	–	–
			Dichloroacetate	21.67	21.67	20.68
			Trifluoroacetate	19.74	19.75	18.50
			Trichloroacetate	–	–	–

Method	Solvation model	Basis Set	Carboxylate	$\Delta E^{\ddagger \text{model}}$ [a]	$\Delta H^{\ddagger \text{model}}$ [b]	$\Delta G^{\ddagger \text{model}}$ [c]
			Heptafluorobutanoate	19.55	19.49	19.76
B97D	IEFPCM	AUG-cc-pVTZ	***Reference Carboxylates***			
			Formate	15.22	15.19	15.08
			Acetate	17.27	17.13	17.14
			2-Methylpropanoate (Isobutyrate)	17.56	17.38	17.67
			2,2-Dimethylpropanoate (Pivalate)	17.62	17.52	17.15
			Fluoroacetate	14.71	14.61	14.27
			Chloroacetate	14.36	14.29	14.07
			Bromoacetate	15.00	14.96	14.43
			Dichloroacetate	13.04	12.95	12.51
			Trifluoroacetate	11.65	11.56	11.33
			Trichloroacetate	11.52	11.46	10.85
			Heptafluorobutanoate	11.27	11.25	10.77
B97D	IEFPCM	6-311+G(3df,2p)	***Reference Carboxylates***			
			Formate	15.57	15.55	15.43
			Acetate	17.59	17.46	17.44
			2-Methylpropanoate (Isobutyrate)	17.90	17.71	18.10
			2,2-Dimethylpropanoate (Pivalate)	17.95	17.85	17.46
			Fluoroacetate	15.08	14.97	14.69
			Chloroacetate	14.73	14.66	14.45
			Bromoacetate	15.33	15.30	14.62
			Dichloroacetate	13.44	13.32	13.22
			Trifluoroacetate	11.99	11.90	11.74
			Trichloroacetate	11.89	11.83	11.27

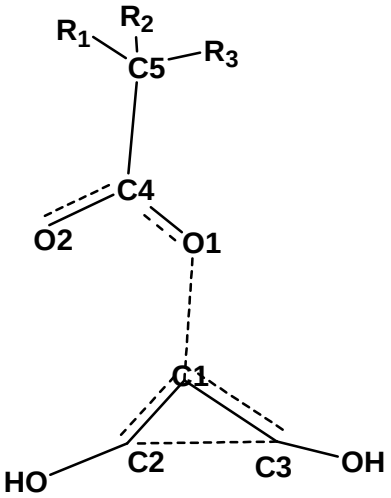
Method	Solvation model	Basis Set	Carboxylate	$\Delta E^{\ddagger \text{model}}$ [a]	$\Delta H^{\ddagger \text{model}}$ [b]	$\Delta G^{\ddagger \text{model}}$ [c]
			Heptafluorobutanoate	11.61	11.58	11.12
M06-2X	SMD	AUG-cc-pVTZ	***Reference Carboxylates***			
			Formate	29.52	29.62	29.11
			Acetate	31.55	31.58	31.21
			2,2-Dimethylpropanoate (Pivalate)	31.57	31.64	30.65
			Fluoroacetate	28.60	28.57	28.27
			Chloroacetate	28.82	28.71	28.72
			Bromoacetate	28.93	28.90	28.49
			Dichloroacetate	26.20	26.20	25.53
			Trifluoroacetate	24.09	23.99	24.08
			Trichloroacetate	24.17	24.10	24.50
			Heptafluorobutanoate	22.96	22.86	23.50
M06-2X	SMD	6-311+G(2d,p)	***Reference Carboxylates***			
			Formate	29.31	29.42	28.91
			Acetate	31.34	31.37	31.04
			2-Methylpropanoate (Isobutyrate)	31.66	31.57	31.50
			2,2-Dimethylpropanoate (Pivalate)	31.47	31.51	30.71
			Fluoroacetate	28.43	28.38	28.15
			Chloroacetate	28.61	28.45	28.62
			Bromoacetate	28.69	28.63	28.35
			Dichloroacetate	25.95	25.94	25.34
			Trifluoroacetate	23.96	23.84	23.95
			Trichloroacetate	23.96	23.92	24.07
			Heptafluorobutanoate	22.80	22.89	22.12

[*a*] Zero-point correction is added to IEFPCM total energy. [*b*] Thermal correction to Enthalpy is added to IEFPCM total energy.
[*c*] Thermal correction to Gibbs Free Energy is added to IEFPCM total energy.

Table S4. Selected geometrical parameters (in angstroms) of *cis*-2,3-dihydroxycyclopropyl carboxylate structures optimized at the M06-2X/AUG-cc-pVTZ level of theory by using IEFPCM solvation model (solvent = water)



Substrate



TS

Carboxylate		**C1–O1**		**C2–C3**		**C1–C2**		**C4–C5**	
		Substrate	TS	Substrate	TS	Substrate	TS	Substrate	TS
Reference Carboxylates									
Formate	HCO_2^-	1.41	1.83	1.52	2.02	1.49	1.40	–	–
Acetate	$CH_3CO_2^-$	1.41	1.84	1.52	2.04	1.49	1.39	1.50	1.52
2-Methylpropanoate (Isobutyrate)	$(CH_3)_2CHCO_2^-$	1.41	1.85	1.52	2.04	1.49	1.39	1.51	1.53
2,2-Dimethylpropanoate (Pivalate)	$(CH_3)_3CCO_2^-$	1.40	1.85	1.52	2.04	1.49	1.39	1.52	1.54
Fluoroacetate	$CH_2FCO_2^-$	1.41	1.82	1.52	2.01	1.49	1.39	1.51	1.52

Carboxylate		**C1–O1**		**C2–C3**		**C1–C2**		**C4–C5**	
		Substrate	TS	Substrate	TS	Substrate	TS	Substrate	TS
Chloroacetate	$CH_2ClCO_2^-$	1.41	1.82	1.52	2.01	1.49	1.40	1.51	1.53
Bromoacetate	$CH_2BrCO_2^-$	1.41	1.82	1.52	2.01	1.49	1.40	1.51	1.53
Dichloroacetate	$CHCl_2CO_2^-$	1.41	1.79	1.52	1.97	1.49	1.40	1.53	1.54
Trifluoroacetate	$CF_3CO_2^-$	1.42	1.79	1.52	1.95	1.49	1.40	1.54	1.55
Trichloroacetate	$CCl_3CO_2^-$	1.41	1.79	1.52	1.96	1.49	1.40	1.55	1.57
Heptafluorobutanoate	$C_3F_7CO_2^-$	1.42	1.78	1.52	1.93	1.49	1.40	1.55	1.55
Other Carboxylates									
Propanoate (Propionate)	$C_2H_5CO_2^-$	1.41	1.85	1.52	2.04	1.49	1.39	1.50	1.52
Butanoate (Butyrate)	$C_3H_7CO_2^-$	1.41	1.84	1.52	2.04	1.49	1.39	1.50	1.52
Phenylacetate	$C_6H_5H_2CO_2^-$	1.41	1.84	1.52	2.03	1.49	1.39	1.51	1.53
Propenoate (Acrylate)	$CH_2{=}CHCO_2^-$	1.41	1.84	1.52	2.03	1.49	1.39	1.48	1.50
Propynoate (Propiolate)	$CH{\equiv}CCO_2^-$	1.41	1.81	1.52	1.99	1.49	1.40	1.45	1.47
Difluoroacetate	$CHF_2CO_2^-$	1.41	1.81	1.52	1.98	1.49	1.40	1.53	1.54
Dibromoacetate	$CHBr_2CO_2^-$	1.41	1.78	1.52	1.96	1.49	1.40	1.52	1.54
Tribromoacetate	$CBr_3CO_2^-$	1.41	1.77	1.52	1.94	1.49	1.40	1.54	1.57
Pentafluoropropanoate	$CF_3CF_2CO_2^-$	1.41	1.79	1.52	1.95	1.49	1.40	1.54	1.56
Pentachloropropanoate	$CCl_3CCl_2CO_2^-$	1.41	1.79	1.52	1.96	1.49	1.40	1.55	1.58
Pentabromopropanoate	$CBr_3CBr_2CO_2^-$	1.41	1.80	1.52	1.96	1.49	1.40	1.55	1.58
Heptachlorobutanoate	$CCl_3CCl_2CCl_2CO_2^-$	1.41	1.79	1.52	1.96	1.49	1.40	1.56	1.59
3,3,3-Trifluoropropanoate	$CF_3CH_2CO_2^-$	1.41	1.82	1.52	2.01	1.49	1.40	1.51	1.53
Hexafluoroisobutanoate	$(CF_3)_2CHCO_2^-$	1.41	1.81	1.52	1.97	1.49	1.40	1.53	1.55
Nonafluorotrimethylacetate	$(CF_3)_3CCO_2^-$	1.42	1.79	1.52	1.94	1.49	1.40	1.55	1.58
Cyanoacetate	$NCCH_2CO_2^-$	1.41	1.81	1.52	1.99	1.49	1.40	1.52	1.54

Carboxylate		**C1–O1**		**C2–C3**		**C1–C2**		**C4–C5**	
		Substrate	TS	Substrate	TS	Substrate	TS	Substrate	TS
Dicyanoacetate	$(NC)_2CHCO_2^-$	1.42	1.79	1.52	1.94	1.49	1.40	1.54	1.57
Tricyanoacetate	$(NC)_3CCO_2^-$	1.42	1.77	1.52	1.89	1.49	1.40	1.58	1.63
Nitroacetate	$O_2NCH_2CO_2^-$	1.41	1.81	1.52	1.98	1.49	1.40	1.52	1.54
Dinitroacetate	$(O_2N)_2CHCO_2^-$	1.42	1.78	1.52	1.93	1.49	1.40	1.53	1.55
Trinitroacetate	$(O_2N)_3CCO_2^-$	1.42	1.76	1.52	1.88	1.49	1.40	1.55	1.59
2-Cyanopropenoate (Cyanoacrylate)	$CH_2=C(CN)CO_2^-$	1.41	1.81	1.52	1.99	1.49	1.40	1.50	1.52
2-Hydroxyethanoate (Glycolate)	$HOCH_2CO_2^-$	1.41	1.82	1.52	2.00	1.49	1.40	1.51	1.52
2-Hydroxypropanoate (Lactate)	$CH_3(HO)CHCO_2^-$	1.41	1.82	1.52	2.01	1.49	1.40	1.51	1.53
2,3-Dihydroxypropanoate (Glycerate)	$HOCH_2(HO)CHCO_2^-$	1.41	1.82	1.52	2.00	1.49	1.40	1.52	1.53
Oxoethanoate (Glyoxylate)	$OHCCO_2^-$	1.41	1.81	1.52	1.98	1.49	1.40	1.53	1.54
2-Oxopropanoate (Pyruvate)	$CH_3C(O)CO_2^-$	1.41	1.81	1.52	1.99	1.49	1.40	1.55	1.56
3-Oxopropanoate (Formylacetate)	$OHCCH_2CO_2^-$	1.41	1.83	1.52	2.02	1.49	1.40	1.50	1.52
2-Oxobutanoate (α-Ketobutyrate)	$CH_3CH_2C(O)CO_2^-$	1.41	1.82	1.52	2.00	1.49	1.40	1.55	1.56
3-Oxobutanoate (Acetoacetate)	$H_3CC(O)CH_2CO_2^-$	1.41	1.84	1.52	2.02	1.49	1.40	1.50	1.52
Oxalate, 1. dissociation	$RO_2CCCO_2^-$	1.41	1.81	1.52	1.98	1.49	1.40	1.54	1.56
Oxalate, 2. dissociation	$^-O_2CCCO_2^-$	1.41	1.84	1.52	2.04	1.48	1.39	1.56	1.54
Malonate, 1. dissociation	$RO_2CCH_2CO_2^-$	1.41	1.83	1.52	2.02	1.49	1.40	1.50	1.52
Malonate, 2. dissociation	$^-O_2CCH_2CO_2^-$	1.40	1.86	1.52	2.05	1.49	1.39	1.49	1.51

II.

Correlations

II.1. Correlations of experimental free energies of activation for solvolyses of dianisylmethyl carboxylates in 80% ethanol against calculated free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates

Calculated free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates ($\Delta G^{\ddagger model}$) are given in Table S3.

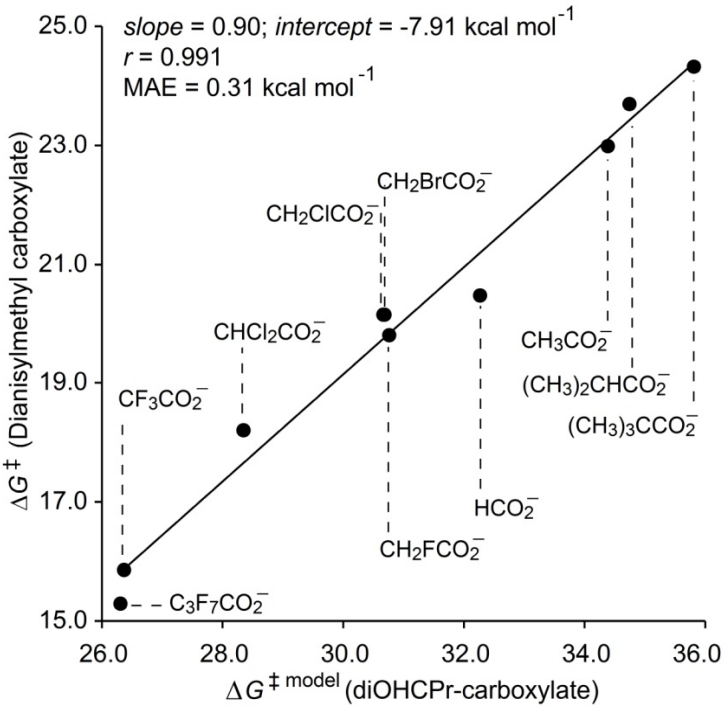


Figure S1. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **M06-2X/AUG-cc-pVDZ** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

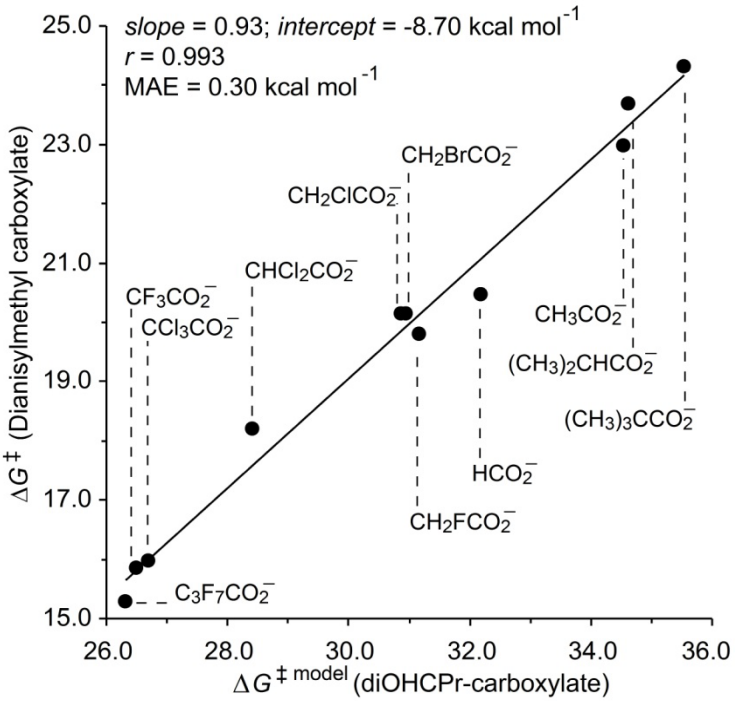


Figure S2. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **M06-2X/6-311+G(3df,2p)** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

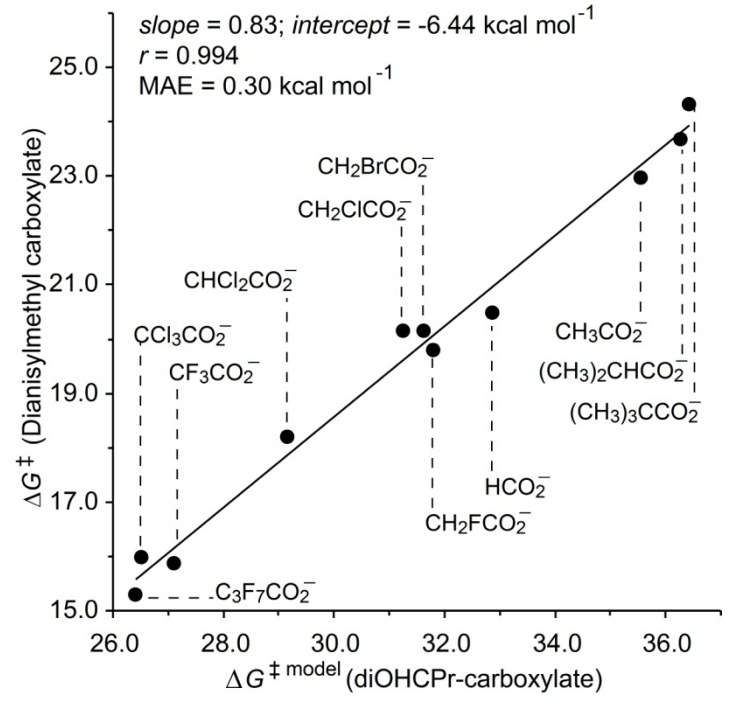


Figure S3. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **M06-2X/6-31+G(d)** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

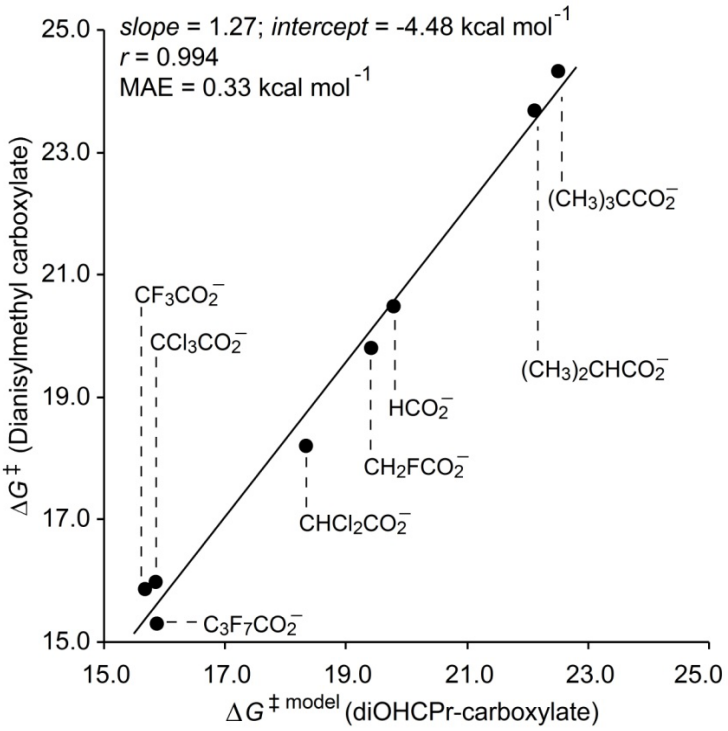


Figure S4. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **B3LYP/AUG-cc-pVTZ** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

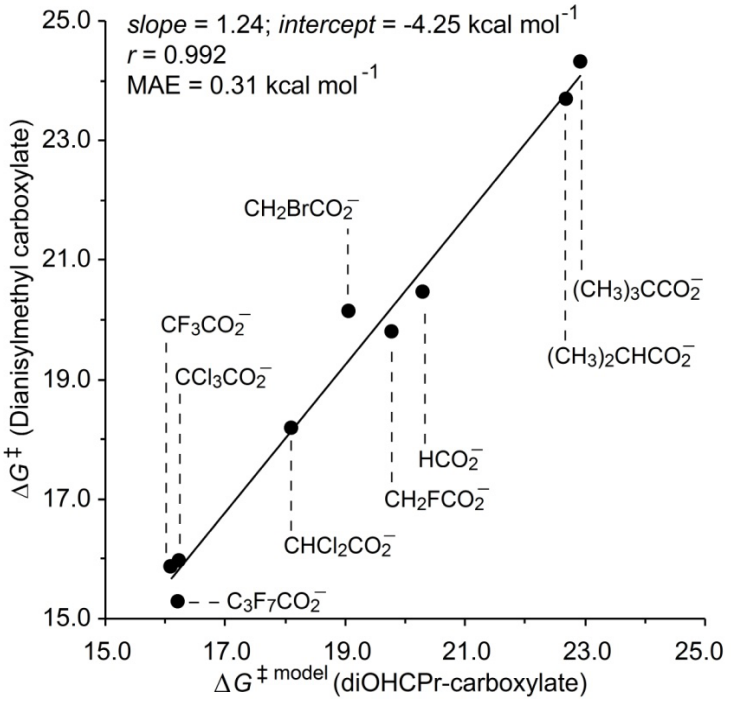


Figure S5. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **B3LYP/6-311+G(3df,2p)** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

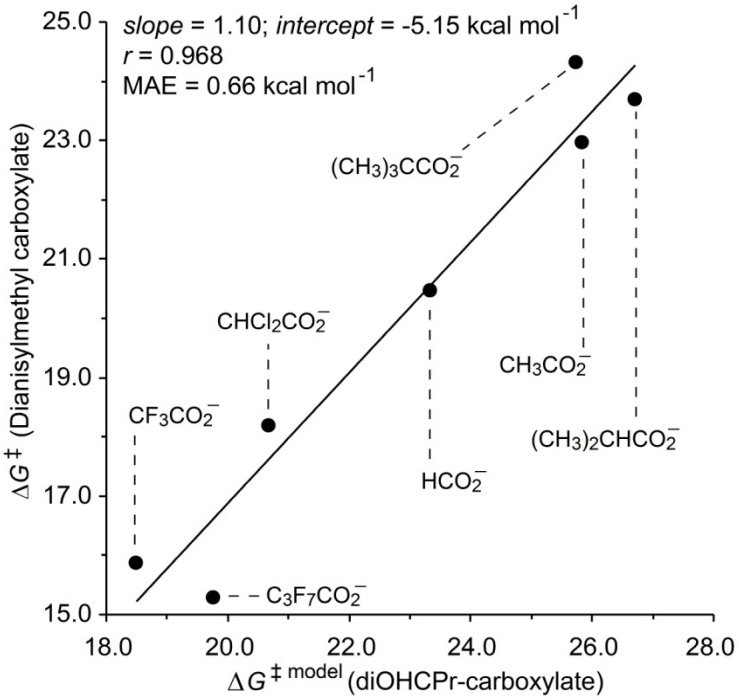


Figure S6. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **mPW3PBE/6-311+G(3df,2p)** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

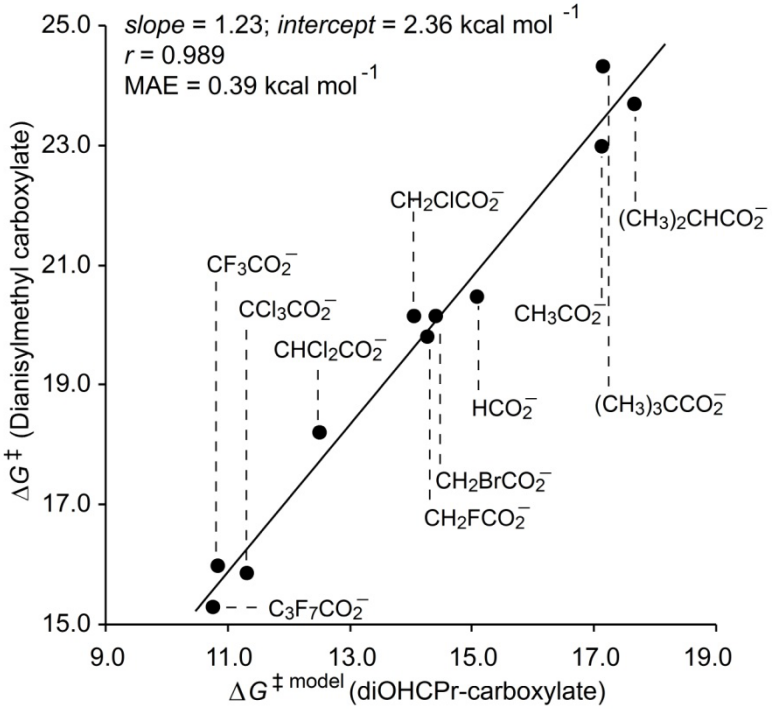


Figure S7. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **B97D/AUG-cc-pVTZ** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

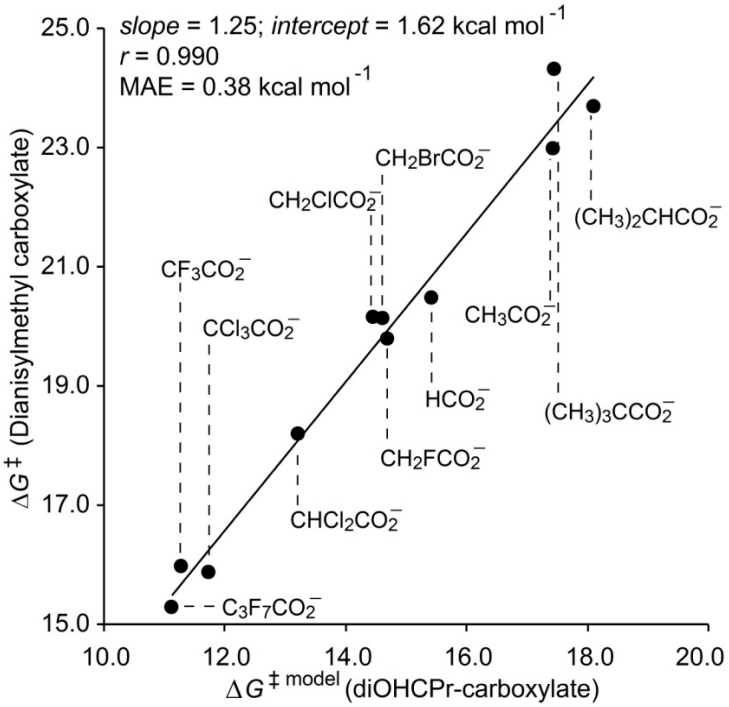


Figure S8. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **B97D/6-311+G(3df,2p)** level of theory in the presence of **IEFPCM** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

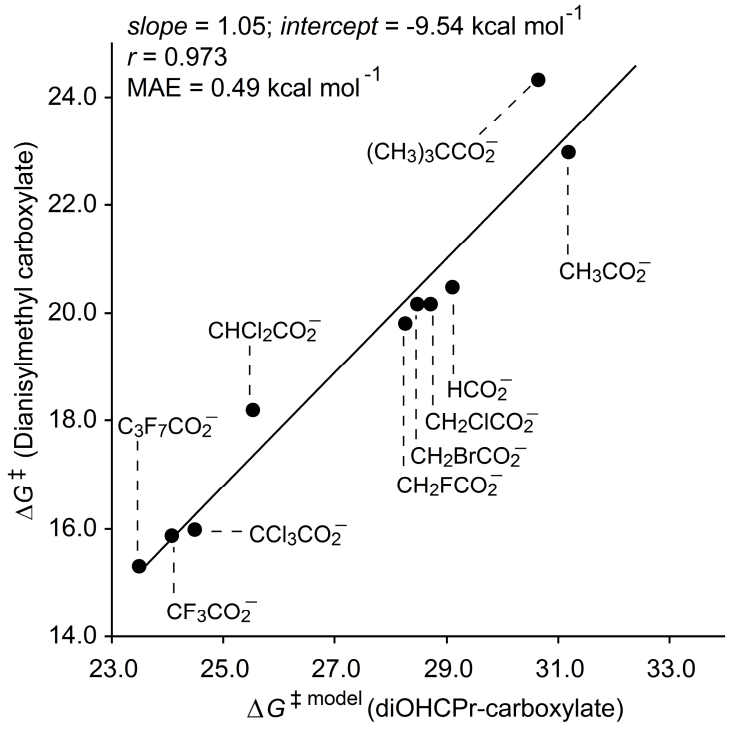


Figure S9. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **M06-2X/AUG-cc-pVTZ** level of theory in the presence of **SMD** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

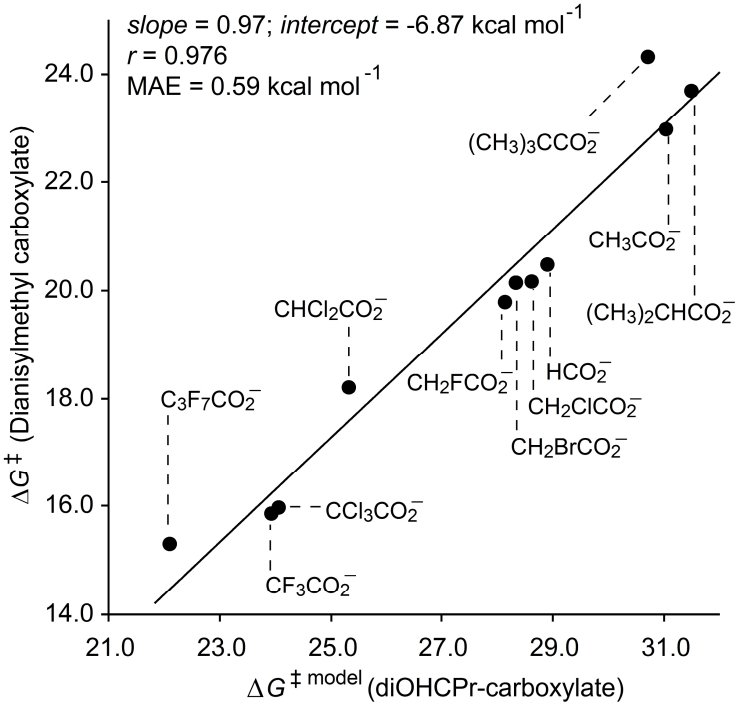


Figure S10. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 80% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the **M06-2X/6-311+G(2d,p)** level of theory in the presence of **SMD** solvation model (solvent = water). The experimental data are taken from references 1 and 2.

II.2. Correlations of experimental free energies of activation for solvolyses of dianisylmethyl carboxylates in aqueous ethanol mixtures against free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the M06-2X/AUG-cc-pVTZ level of theory in the presence of IEFPCM solvation model (solvent = water)

Calculated free energies of activation for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates ($\Delta G^{\ddagger model}$) are given in Table S3.

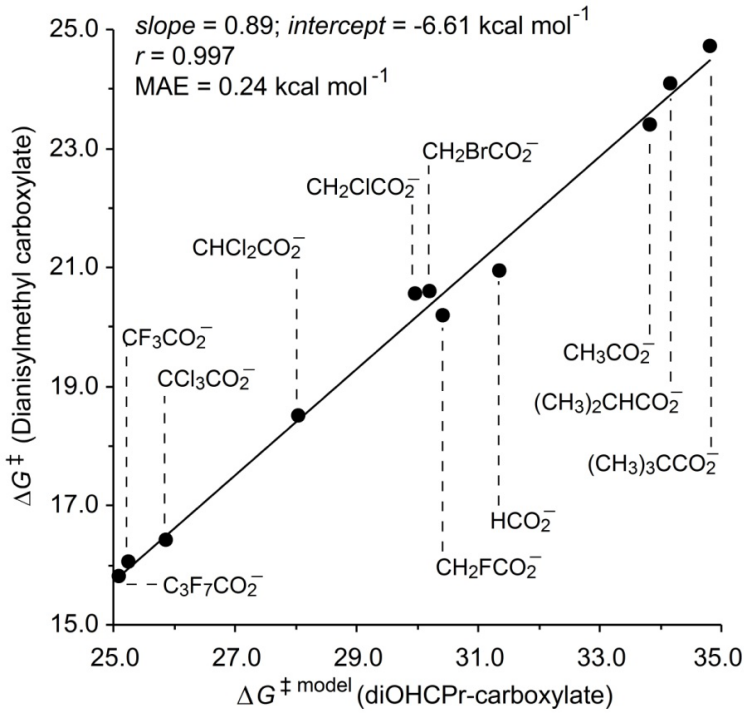


Figure S11. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 90% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the M06-2X/AUG-cc-pVTZ level of theory in the presence of IEFPCM solvation model (solvent = water). The experimental data are taken from references 1 and 2.

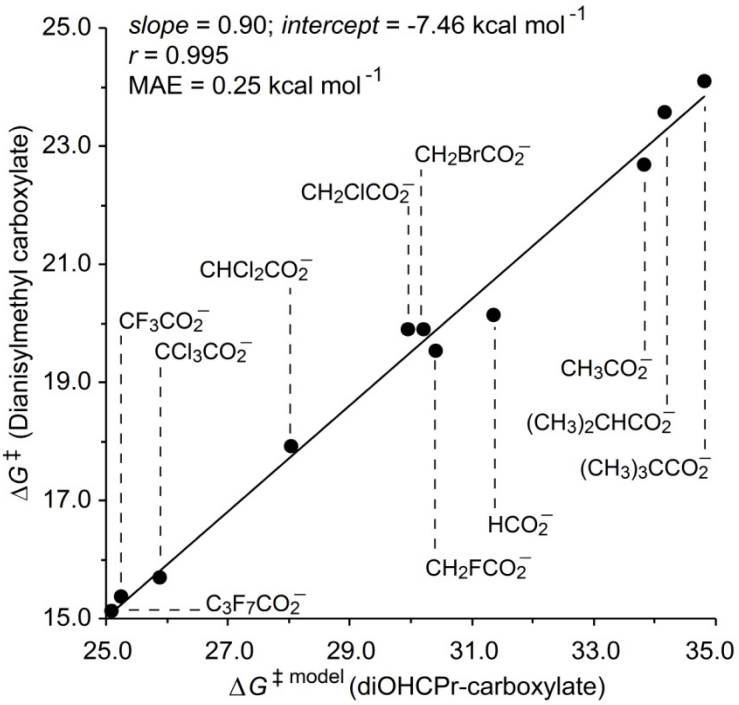


Figure S12. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 70% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the M06-2X/AUG-cc-pVTZ level of theory in the presence of IEFPCM solvation model (solvent = water). The experimental data are taken from references 1 and 2.

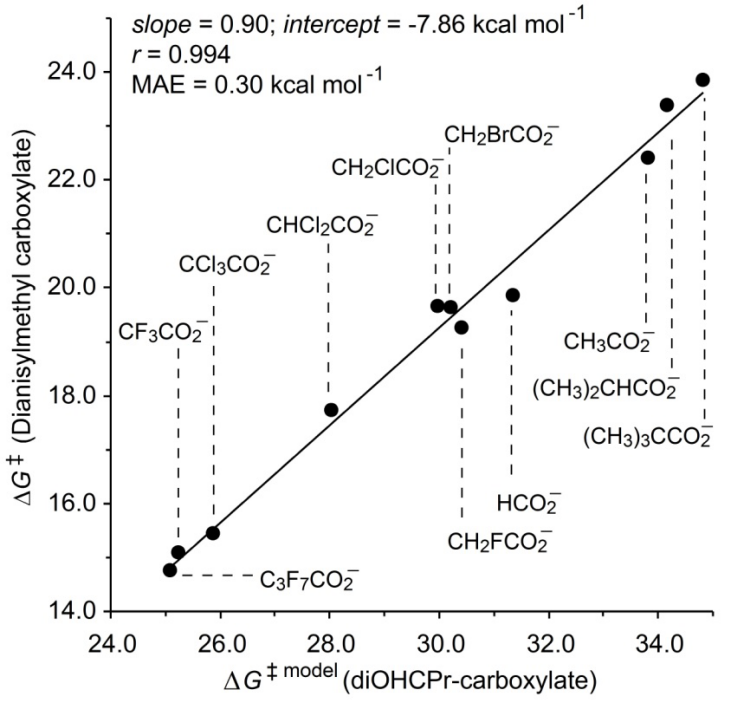
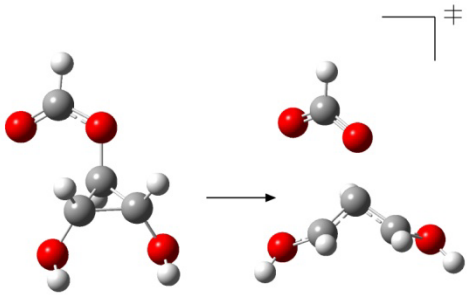
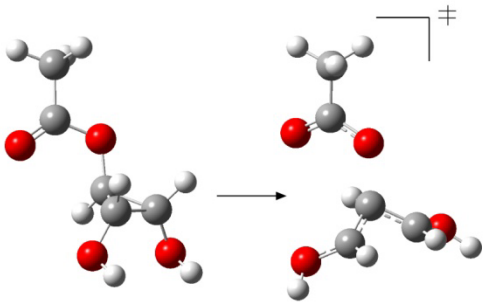


Figure S13. Correlation of experimental free energies of activation (in kcal mol^{-1}) for solvolyses of dianisylmethyl carboxylates in 60% ethanol against free energies of activation (in kcal mol^{-1}) for heterolysis of *cis*-2,3-dihydroxycyclopropyl carboxylates calculated at the M06-2X/AUG-cc-pVTZ level of theory in the presence of IEFPCM solvation model (solvent = water). The experimental data are taken from references 1 and 2.

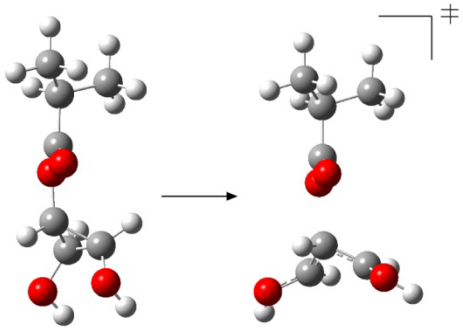
III.
Geometries of *cis*-2,3-dihydroxycyclopropyl carboxylates and geometries of related heterolytic transition states optimized at the IEFPCM-M06-2X/AUG-cc-pVTZ level



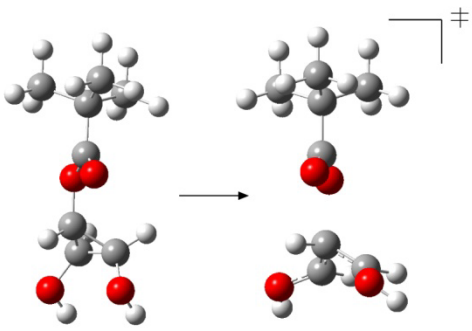
diOHCPr - Formate



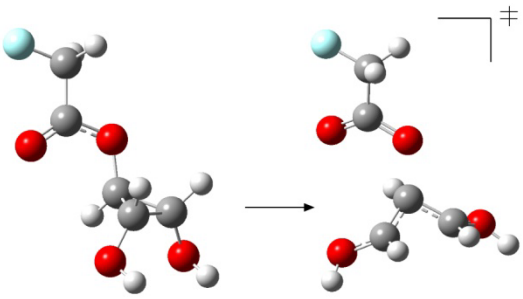
diOHCPr - Acetate



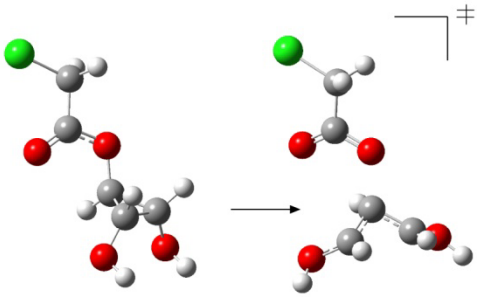
diOHCPr - 2-Methylpropanoate



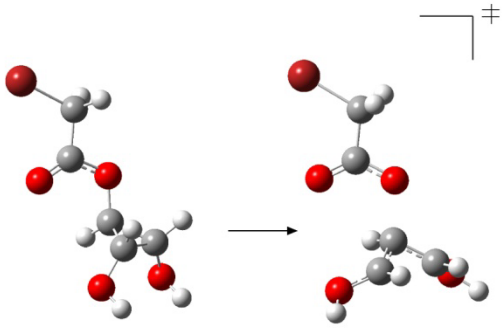
diOHCPr - 2,2-Dimethylpropanoate



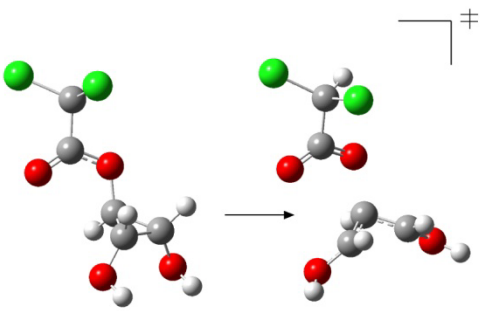
diOHCPr - Fluoroacetate



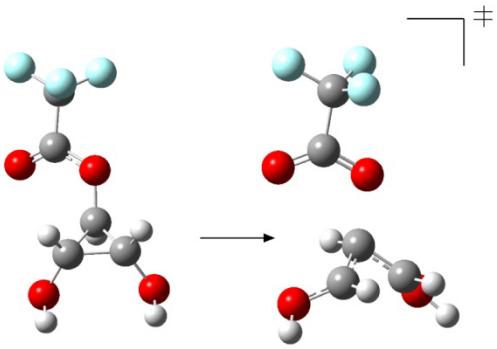
diOHCPr - Chloroacetate



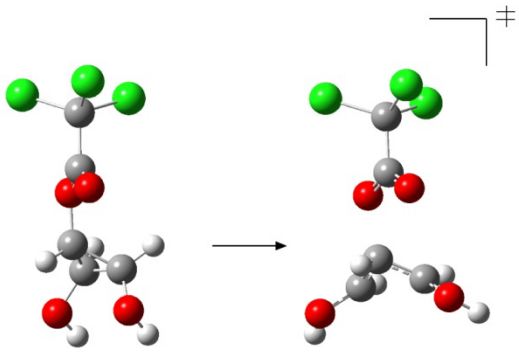
diOHCPr - Bromoacetate



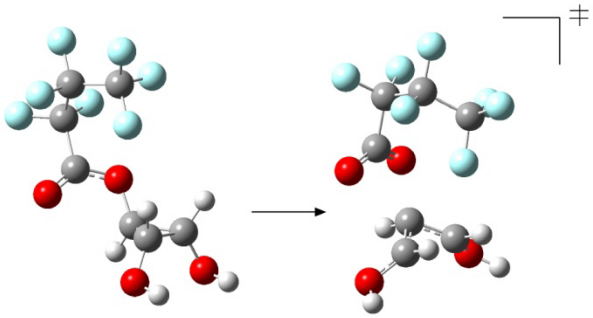
diOHCPr - Dichloroacetate



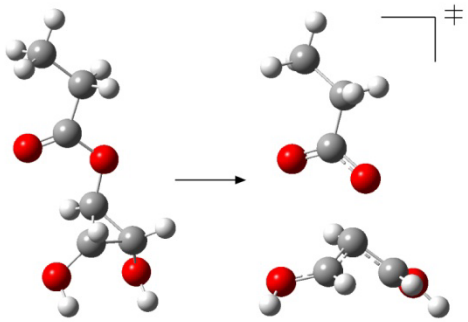
diOHCPr - Trifluoroacetate



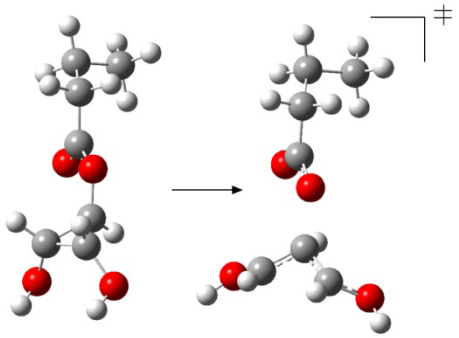
diOHCPr - Trichloroacetate



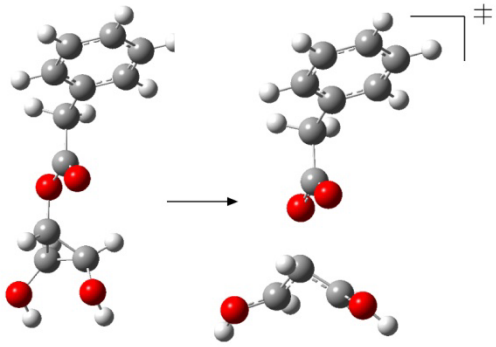
diOHCPr - Heptafluorobutanoate



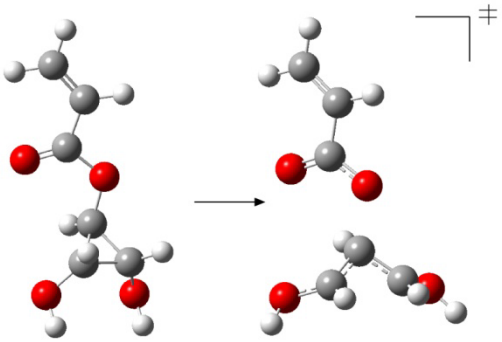
diOHCPr - Propanoate



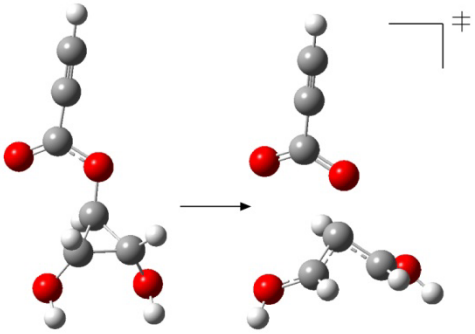
diOHCPr - Butanoate



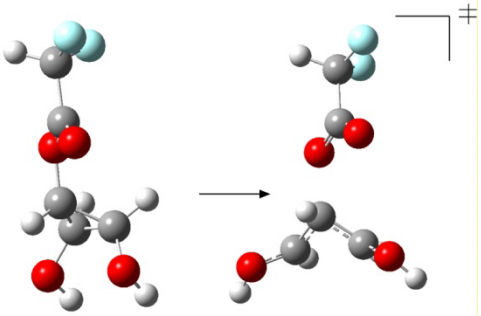
diOHCPr - Phenylacetate



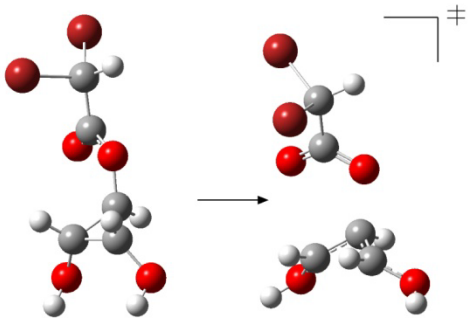
diOHCPr - Propenoate



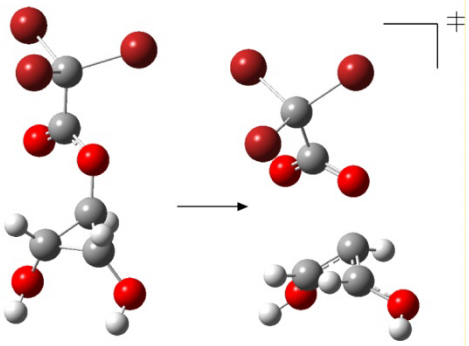
diOHCPr - Propynoate



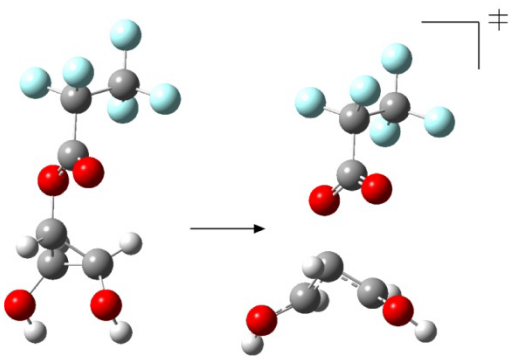
diOHCPr - Difluoroacetate



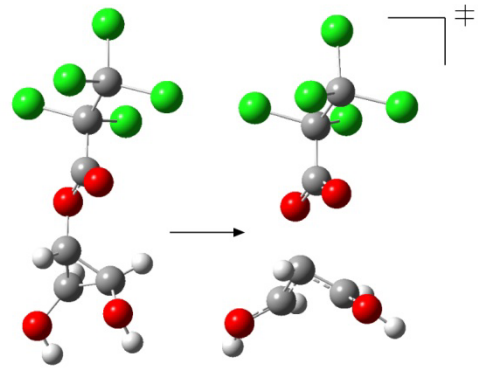
diOHCPr - Dibromoacetate



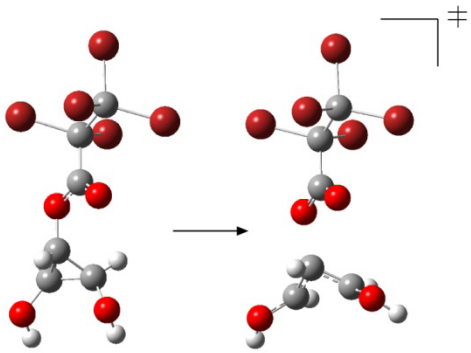
diOHCPr - Tribromoacetate



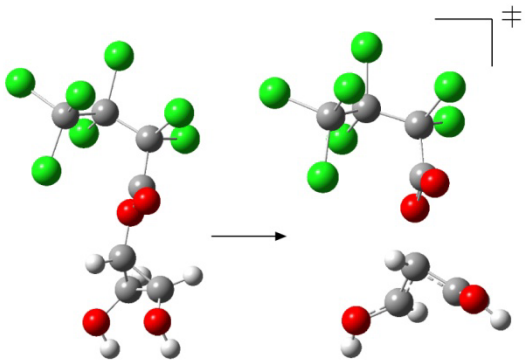
diOHCPr - Pentafluoropropanoate



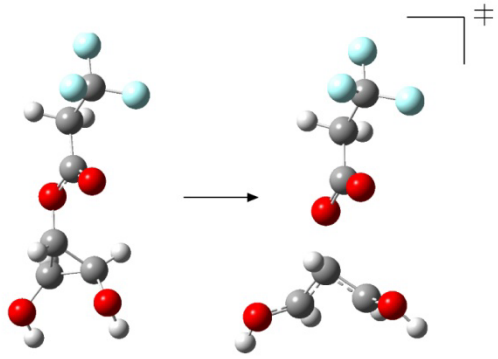
diOHCPr - Pentachloropropanoate



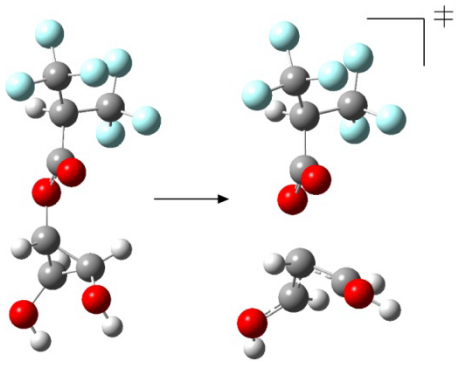
diOHCPr - Pentabromopropanoate



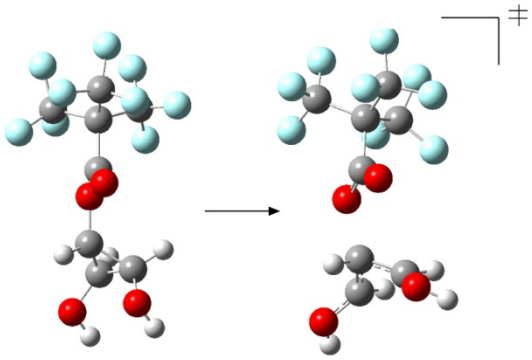
diOHCPr - Heptachlorobutanoate



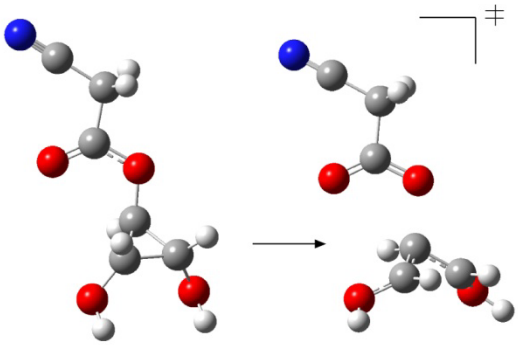
diOHCPr - 3,3,3-Trifluoropropanoate



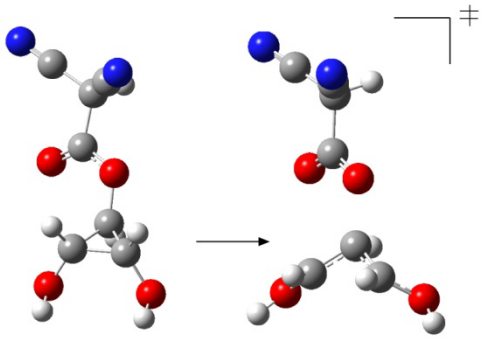
diOHCPr - Hexafluoroisobutanoate



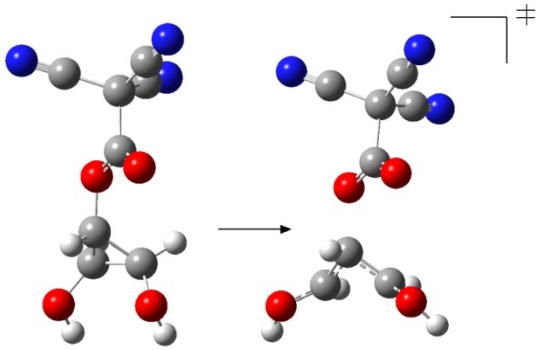
diOHCPr - Nonafluorotrimethylacetate



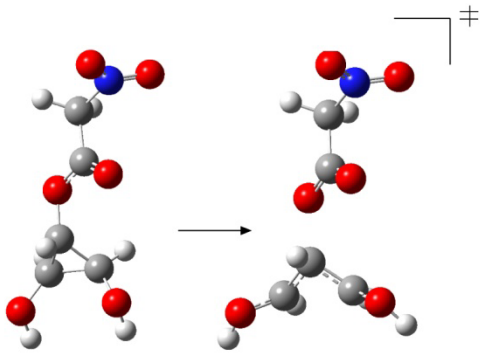
diOHCPr - Cyanoacetate



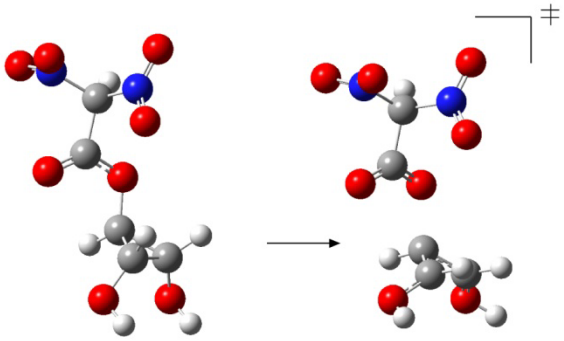
diOHCPr - Dicyanoacetate



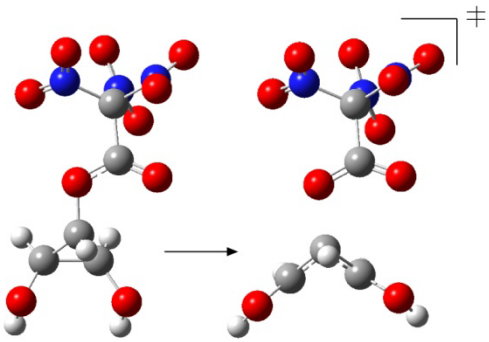
diOHCPr - Tricyanoacetate



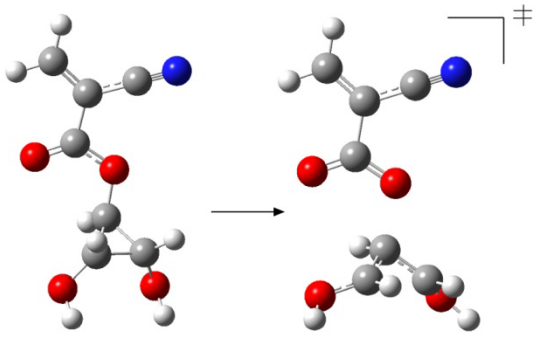
diOHCPr - Nitroacetate



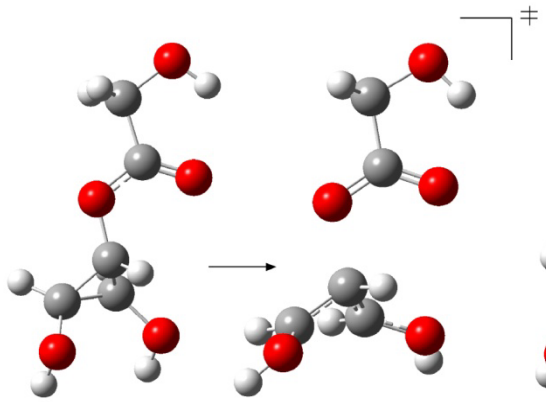
diOHCPr - Dinitroacetate



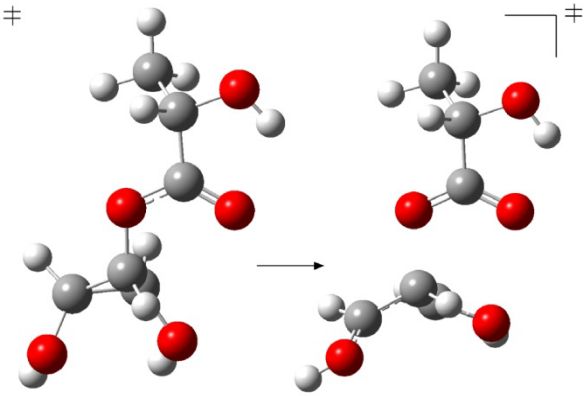
diOHCPr - Trinitroacetate



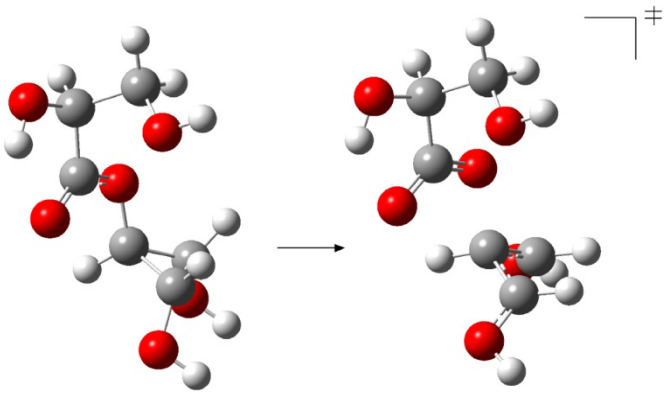
diOHCPr - 2-Cyanopropenoate



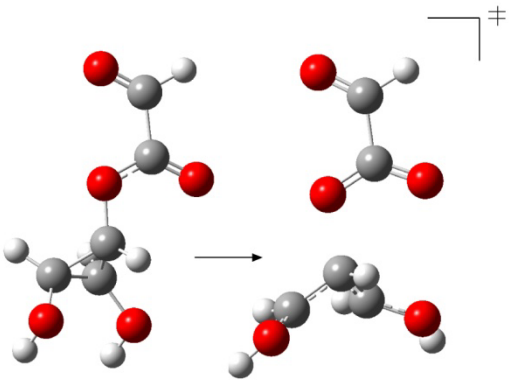
diOHCPr - 2-Hydroxyethanoate (Glycolate)



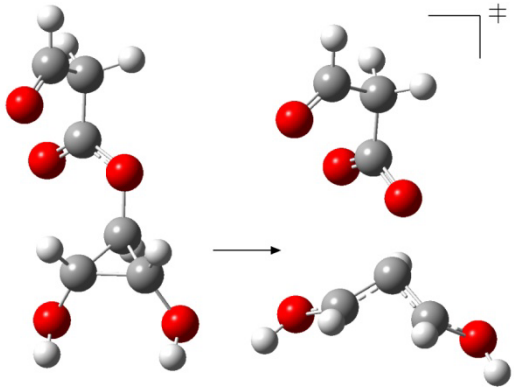
diOHCPr - 2-Hydroxypropanoate (Lactate)



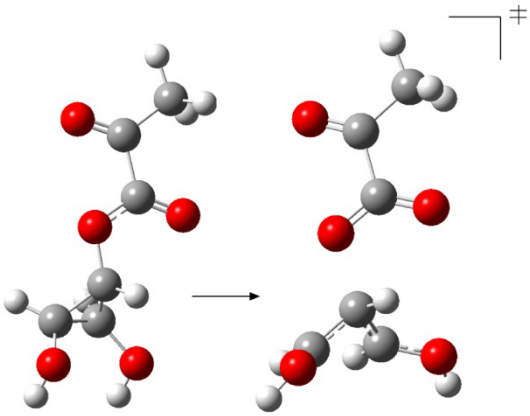
diOHCPr - 2,3-Dihydroxypropanoate (Glycerate)



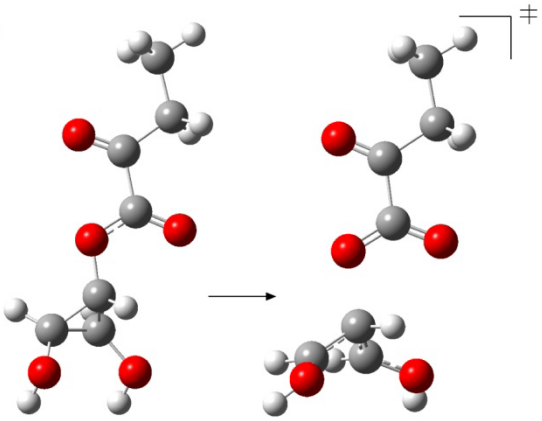
diOHCPr - 2-Oxoethanoate (Glyoxylate)



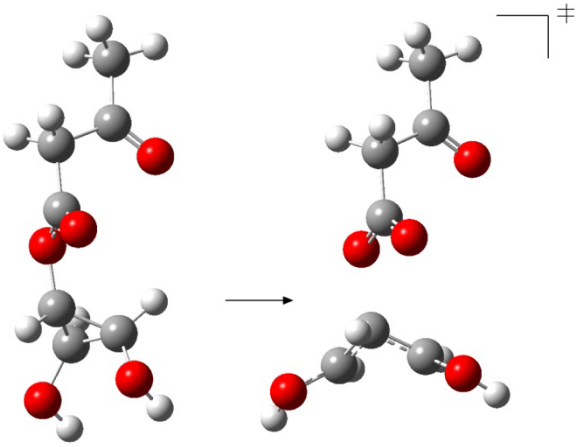
diOHCPr - 3-Oxopropanoate (Formylacetate)



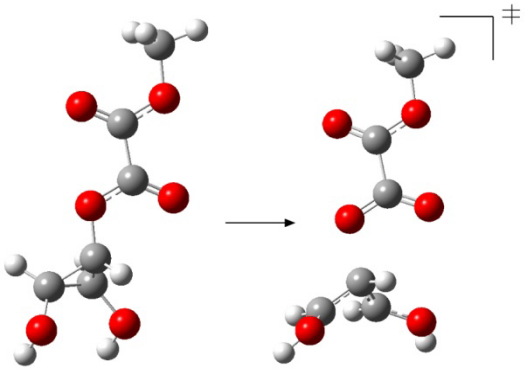
diOHCPr - 2-Oxopropanoate (Pyruvate)



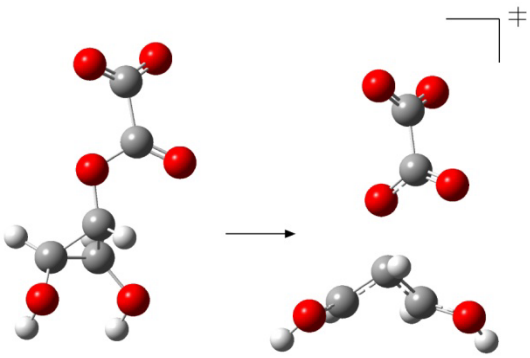
diOHCPr - 2-Oxobutanoate (α -Ketobutyrate)



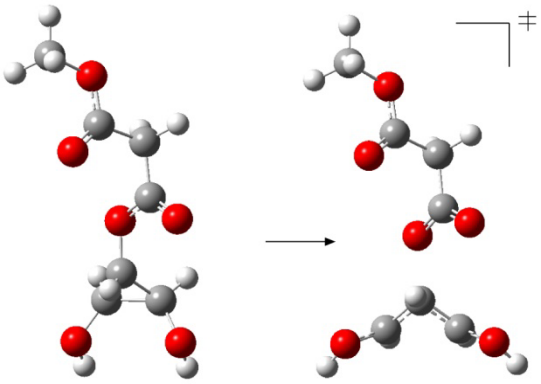
diOHCPr - 3-Oxobutanoate (Acetoacetate)



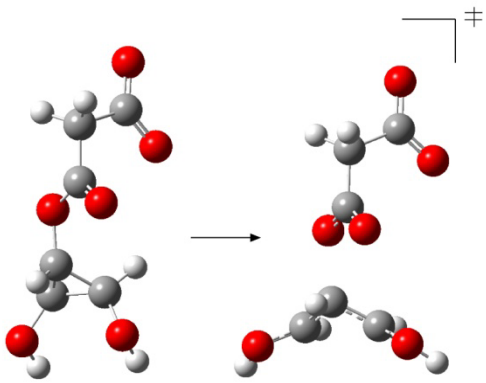
diOHCPr - Oxalate, 1. dissociation



diOHCPr - Oxalate, 2. dissociation



diOHCPr - Malonate, 1. dissociation



diOHCPr - Malonate, 2. dissociation

IV.
Coordinates and energies

M06-2X/AUG-cc-pVTZ
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.903314
E (total electronic) + ZPVE = -456.797416
Internal Thermal Energy = -456.789161
Enthalpy = -456.788216
Gibbs Free Energy = -456.830697

C,0,-0.8220009104,-0.2445480315,-0.3500869389
C,0,-2.0111406004,-0.8294106291,0.3144620994
C,0,1.4808897626,0.0276708693,-0.165762851
O,0,1.427054634,1.1418064978,-0.6033354952
O,0,0.4324634234,-0.7809602017,0.0056634471
C,0,-1.5701324568,0.5858295315,0.6335325096
O,0,-2.2570463277,1.6701600914,0.1033846777
O,0,-3.1121881574,-1.0534036729,-0.5027381803
H,0,-0.9256835389,0.0358723004,-1.3895141111
H,0,-1.8256091092,-1.5648535671,1.088545979
H,0,-1.112473901,0.7299634592,1.6054821488
H,0,-3.0756832811,1.7929662233,0.5946829163
H,0,-3.9143283032,-0.9259110809,0.0138489197
H,0,2.396949246,-0.4794127896,0.147805249

TS–diOHCPr-Formate
E (total electronic) = -456.8494857
E (total electronic) + ZPVE = -456.746352
Internal Thermal Energy = -456.737790
Enthalpy = -456.736846
Gibbs Free Energy = -456.780724

C,0,-1.2067375881,-0.076632768,-0.0682877642
C,0,-2.3103214851,-0.8541788588,0.2829592213
C,0,-1.7269815883,1.0581855462,0.5553764639
O,0,-1.7092665989,2.2324801784,-0.0777599676
O,0,-2.8862814835,-1.6384207498,-0.6319741038
H,0,-0.9810345845,0.0121009005,-1.1217500923
H,0,-2.6532743241,-0.9374686078,1.3040155496
H,0,-2.0432517984,1.048410999,1.5884055842
H,0,-2.1882315566,2.9007636851,0.4253993373
H,0,-3.6947880739,-2.033084561,-0.286311245
C,0,1.4317002636,-0.1320673957,-0.0713709054
O,0,1.4006427707,0.8197435596,-0.8426394258
O,0,0.4263409008,-0.7349975628,0.4479855062
H,0,2.4046973963,-0.5524145051,0.2413428916

diOHCPr-Acetate
E (total electronic) = -496.2230482
E (total electronic) + ZPVE = -496.089704
Internal Thermal Energy = -496.079691
Enthalpy = -496.078747
Gibbs Free Energy = -496.125787

C,0,-0.8195207164,-0.2532937086,-0.3453503364
C,0,-2.0153544638,-0.8313888283,0.3150277792
C,0,2.758363244,-0.6617910328,0.2674290526
C,0,1.4920663843,0.0115669139,-0.1583072159
O,0,1.3976727637,1.1249344454,-0.6043423719
O,0,0.4267915123,-0.7965699448,0.0122265241
C,0,-1.566916776,0.5808022093,0.6355227196
O,0,-2.2497366657,1.6686555361,0.1055213059
O,0,-3.1165827538,-1.0463060334,-0.5055915603
H,0,-0.9231457395,0.0282631825,-1.3846880121
H,0,-1.8390083358,-1.5691137361,1.0890856794
H,0,2.682212201,-0.9465853234,1.3154425309
H,0,2.897694408,-1.5714925413,-0.3141605144
H,0,-1.1113905619,0.7228773374,1.608858833
H,0,-3.0724965763,1.7879921198,0.5905563965
H,0,-3.9189575852,-0.8907804404,0.0026136804
H,0,3.5968221512,0.0094977446,0.1202470094

TS–diOHCPr-Acetate
E (total electronic) = -496.1657279
E (total electronic) + ZPVE = -496.034645
Internal Thermal Energy = -496.024515
Enthalpy = -496.023571
Gibbs Free Energy = -496.071876

C,0,-0.5603288304,-1.1087260164,-0.520749433
C,0,-1.0427392293,-1.7030860552,-1.6858938095
C,0,0.6064091631,-1.8722583982,-0.5029249938
O,0,1.0239362666,-2.4232622708,0.6371933042
O,0,-2.3211481608,-2.0789064592,-1.7590389909
H,0,-1.1851979371,-1.1542523396,0.3600152689
H,0,-0.4443369465,-1.7792842023,-2.582282186
H,0,1.2540127842,-1.9487973527,-1.3647692379
H,0,1.7824498823,-2.9980713636,0.4842832225
H,0,-2.4927748515,-2.562078237,-2.5752925663
C,0,-0.3452878095,2.8252260927,0.5050397579
C,0,-0.3963161663,1.3117753922,0.5784056704
O,0,-0.4149707792,0.7306487341,1.6637366645
O,0,-0.4214248279,0.7254794787,-0.5704900166
H,0,0.5053028,3.1338614478,-0.1005085875
H,0,-1.246515158,3.190763396,0.0140907835
H,0,-0.2692871995,3.2554951534,1.4990971493

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.8390175
E (total electronic) + ZPVE = -574.648611
Internal Thermal Energy = -574.635971
Enthalpy = -574.635027
Gibbs Free Energy = -574.688545

C,0,-1.1270235604,-0.001979562,-0.4994794908
C,0,-2.2498593529,-0.8929740039,-0.1169455181
C,0,2.4962533776,-0.4433806677,-0.1917114771
C,0,1.1817198146,0.2862319904,-0.3008487187
O,0,1.0216526262,1.4744947204,-0.1976541329
O,0,0.1585989516,-0.5699809926,-0.4962553709
C,0,-1.8202775091,0.2389454033,0.7955649181

O,0,-2.5762618825,1.4021860141,0.8712056917
O,0,-3.4051605416,-0.7745907646,-0.8807628409
C,0,3.6651896062,0.4949041003,-0.4458224162
C,0,2.5755552877,-1.079608984,1.2018949759
H,0,-1.3177543276,0.7173821563,-1.2845018802
H,0,-1.9913610101,-1.8915057679,0.2157839768
H,0,2.4810685629,-1.2405701621,-0.9357024653
H,0,-1.2916453126,-0.0544802554,1.6956980168
H,0,-3.3542185408,1.2351106868,1.4128922121
H,0,-4.1697127426,-0.9195813771,-0.314306098
H,0,3.6881854336,1.2850065142,0.3040291697
H,0,4.6000382056,-0.0606718696,-0.3887492216
H,0,3.5972624576,0.9593546146,-1.4283778229
H,0,1.7462754748,-1.7626566355,1.3767613128
H,0,3.5077399866,-1.634350465,1.2955184442
H,0,2.5603099952,-0.3057176931,1.9704397358

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.7811191
E (total electronic) + ZPVE = -574.593051
Internal Thermal Energy = -574.580372
Enthalpy = -574.579428
Gibbs Free Energy = -574.634092

C,0,-1.5441356766,-0.0882953,-0.0884639384
C,0,-2.5981168937,-0.8496937311,0.4133443001
C,0,-2.0348493543,1.1125677847,0.4224806352
O,0,-2.0440345658,2.2069616384,-0.3377808195
O,0,-3.1803020845,-1.7690093585,-0.3583353945
C,0,2.5033054694,-0.5317351816,0.2401090896
C,0,1.1125342983,-0.1357731115,-0.2518107048
O,0,0.9750985798,0.6491598617,-1.1908366258
O,0,0.1405210837,-0.6504412052,0.4211218896
C,0,3.5429104892,-0.4673923629,-0.8683298408
C,0,2.8770420092,0.395746947,1.3997742915
H,0,-1.3603716015,-0.1260369723,-1.1526442555
H,0,-2.9027868156,-0.7976717383,1.4487928822
H,0,-2.3199312756,1.219512131,1.4593786355
H,0,-2.4993982014,2.9306444904,0.1073036641
H,0,-3.9548588971,-2.1427352486,0.0769411778
H,0,2.4305014318,-1.550427883,0.6225329364
H,0,4.514727837,-0.7849005846,-0.4894314083
H,0,3.2737322117,-1.1101346914,-1.7061893294
H,0,3.6360439454,0.5517998864,-1.2419472509
H,0,3.8525723199,0.1230651004,1.802306407
H,0,2.931509861,1.4287640018,1.0515230283
H,0,2.1444297968,0.3398725425,2.2039958517

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.148236
E (total electronic) + ZPVE = -613.930081
Internal Thermal Energy = -613.916093
Enthalpy = -613.915148
Gibbs Free Energy = -613.971498

C,0,-1.3309760921,-0.1598302088,-0.4105197452
C,0,-2.4153908513,-0.8896973462,0.2907149636
C,0,2.3142437285,-0.1277989572,0.0798768792
C,0,0.9382581276,0.3807448686,-0.3104325971
O,0,0.6846487026,1.4778168929,-0.7355538415
O,0,-0.0142371484,-0.5546853705,-0.1212574673
C,0,-2.1231128355,0.5601399208,0.6240467707
O,0,-2.9572048464,1.5674983384,0.1546498218
O,0,-3.5228266715,-1.2197002807,-0.4819914301
C,0,2.6338876789,-1.3883095801,-0.7323621362
C,0,3.3456313562,0.9580273194,-0.2048121446
C,0,2.2979881864,-0.4624254077,1.5771070817
H,0,-1.5177200548,0.126138473,-1.4369317962
H,0,-2.1144988807,-1.615338092,1.0373942145
H,0,-1.6384989248,0.7377343153,1.5775504116
H,0,-3.7628617211,1.5782990355,0.6812923166
H,0,-4.3115533844,-1.1715826661,0.0674886686
H,0,3.6338218825,-1.7336826371,-0.4690057609
H,0,1.9245128146,-2.1855426854,-0.5193341955
H,0,2.6159455625,-1.1798802573,-1.8026509394
H,0,3.1310712873,1.8615429299,0.3643205041
H,0,4.3338114879,0.5958404452,0.0782706754
H,0,3.3610768594,1.2162485582,-1.2630720944
H,0,3.2915537971,-0.7973337027,1.8756765121
H,0,2.0404809049,0.4150455736,2.1715251629
H,0,1.5848273944,-1.2551456782,1.7957267914

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.0902586
E (total electronic) + ZPVE = -613.874227
Internal Thermal Energy = -613.860364
Enthalpy = -613.859420
Gibbs Free Energy = -613.916009

C,0,-1.7510347764,-0.0642037328,-0.0955818922
C,0,-2.6894307667,-1.0183790183,0.2937489959
C,0,-2.3997491948,0.9869811189,0.550840638
O,0,-2.5572519319,2.1555353055,-0.0695741379
O,0,-3.1386082338,-1.9083982085,-0.5928161708
H,0,-1.5664002545,0.0542142455,-1.1537788915
H,0,-2.9993418413,-1.1335224547,1.3224798669
H,0,-2.6945434668,0.924738813,1.5887690722
H,0,-3.1032892416,2.7533915957,0.4534636892
H,0,-3.8535530156,-2.4366613354,-0.2200197062
C,0,2.3425242306,-0.136763665,0.0824919207
C,0,0.8888480602,0.2442262007,-0.2527574974
O,0,0.6365196301,1.1407712449,-1.058341294
O,0,-0.0050760862,-0.4535419077,0.3605157074
C,0,3.3144728465,0.8279641107,-0.5869773824
C,0,2.5891132849,-1.5589235215,-0.4324529957
C,0,2.5374996874,-0.1002855543,1.6001440421
H,0,4.3389512476,0.5430147255,-0.3414866961
H,0,3.2005863995,0.8113084502,-1.6700519788
H,0,3.149814516,1.8499399336,-0.2458646763
H,0,3.617559995,-1.854095542,-0.2173666488
H,0,1.9169268485,-2.268170297,0.0482097447
H,0,2.4390976111,-1.6144352143,-1.5121125742
H,0,3.5674957172,-0.3661596497,1.8439496473
H,0,2.3425856373,0.8983228648,1.9952798563
H,0,1.8700951375,-0.8032187678,2.0950489815

diOHCPr-Fluoroacetate

E (total electronic) = -595.4650534
E (total electronic) + ZPVE = -595.338439
Internal Thermal Energy = -595.327894
Enthalpy = -595.326949
Gibbs Free Energy = -595.375658

C,0,0.2360180192,-0.9445122029,-0.1893289955
C,0,0.8736643114,-1.4889162921,1.0332991563
C,0,-0.8505351448,2.4290617977,-1.043708928
C,0,-0.8538705737,0.9190141505,-1.0627961847
O,0,-1.6128214973,0.2338660491,-1.68603873
O,0,0.1274906434,0.4581050857,-0.2793444947
C,0,-0.6095740657,-1.6851212851,0.786680611
O,0,-1.0916151848,-2.9124697496,0.3515974916
O,0,1.7629150263,-2.5372593016,0.833580154
F,0,-1.8549857855,2.9010599827,-1.8493005115
H,0,0.4467146613,-1.4496958092,-1.1220953438
H,0,1.1301447761,-0.7774032354,1.8094617931
H,0,-1.0084793768,2.7798535783,-0.0243665087
H,0,0.1085958773,2.7955062327,-1.4079542247
H,0,-1.2727464561,-1.0965440219,1.4102545792
H,0,-1.1087361981,-3.5233659235,1.095286697
H,0,1.7137589676,-3.1357260554,1.5858014397

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.4133974
E (total electronic) + ZPVE = -595.288915
Internal Thermal Energy = -595.278344
Enthalpy = -595.277400
Gibbs Free Energy = -595.327185

C,0,0.0146700016,-1.3009233608,-0.1266562688
C,0,-1.0076833433,-1.8035820767,-0.9322873503
C,0,0.9950044667,-1.9265644863,-0.8989561945
O,0,1.970595635,-2.6162068137,-0.303565522
O,0,-2.0815394817,-2.3642848955,-0.3677407546
H,0,-0.0114149331,-1.5631735758,0.9218278101
H,0,-1.023734757,-1.6505784759,-2.0014931475
H,0,1.0656263487,-1.7739962838,-1.9662769195
H,0,2.5118102937,-3.0760547313,-0.9552333848
H,0,-2.6501333524,-2.7642076928,-1.0353253487
C,0,0.8728749371,2.4370828572,1.1079825052
C,0,0.8865770676,0.9197328115,0.9778480457
O,0,1.6305900187,0.2292412907,1.6587936244
O,0,0.0472184405,0.508689878,0.0949199286
F,0,1.7844027859,2.8689344857,2.0512225261
H,0,1.1264430374,2.8853738193,0.1482867364
H,0,-0.1209011655,2.7663342502,1.4086687143

diOHCPr-Chloroacetate

E (total electronic) = -955.8261973
E (total electronic) + ZPVE = -955.701252
Internal Thermal Energy = -955.690444
Enthalpy = -955.689500
Gibbs Free Energy = -955.739459

C,0,-0.073701936,-1.0420987269,0.3278612068
C,0,-0.8287600105,-1.8227634232,-0.6812739968
C,0,0.558331905,2.5299719988,0.607402581
C,0,0.8382723885,1.0542308282,0.7742733004
O,0,1.8035816772,0.5591507143,1.2794827799
O,0,-0.187953693,0.3614120799,0.2620795268
C,0,0.6861133992,-1.767468093,-0.7265080223
O,0,1.4415733038,-2.8459593536,-0.2857680097
O,0,-1.4766301468,-2.9557795481,-0.2056460813
Cl,0,1.8594299568,3.533714106,1.2655001103
H,0,-0.0176027455,-1.4519051284,1.3271766801
H,0,-1.341656206,-1.2593571471,-1.451975646
H,0,0.4451520065,2.7541739455,-0.4494231324
H,0,-0.3667711364,2.7784811253,1.1193815108
H,0,1.1116396658,-1.1709660009,-1.5253614237
H,0,1.4323718612,-3.5316089895,-0.9612927212
H,0,-1.47308029,-3.6289593871,-0.8936046626

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.7748219
E (total electronic) + ZPVE = -955.652056
Internal Thermal Energy = -955.641174
Enthalpy = -955.640229
Gibbs Free Energy = -955.691697

C,0,0.0224586263,-1.3397021339,-0.2525320804
C,0,-1.006690659,-1.8316011446,-1.0564540427
C,0,0.9938673537,-1.9701166067,-1.0326040679
O,0,1.9656311819,-2.6724271317,-0.4455003074
O,0,-2.0815851227,-2.3884169329,-0.489966211
H,0,-0.0011223483,-1.6074025851,0.7947246215
H,0,-1.0268817987,-1.6725128158,-2.124682001
H,0,1.0616213501,-1.8118195627,-2.099250756
H,0,2.4993684277,-3.133700845,-1.1023049218
H,0,-2.6557355984,-2.7807906361,-1.1572446686
C,0,0.8805322195,2.3923547873,0.9785591499
C,0,0.9067614214,0.8683371139,0.8657257791
O,0,1.6379635362,0.16722158,1.5462928732
O,0,0.0694945665,0.4658747227,-0.0245063059
Cl,0,2.0306822646,3.0431524552,2.1759666029
H,0,1.1244920656,2.827342789,0.0145435635
H,0,-0.1153004862,2.7128679466,1.2681797723

diOHCPr-Bromoacetate

E (total electronic) = -3069.860866
E (total electronic)+ZPVE = -3069.736530
Internal Thermal Energy = -3069.725553
Enthalpy = -3069.724608
Gibbs Free Energy = -3069.776004

C,0,-0.1299559444,-1.0820032133,0.3290585348
C,0,-0.8920795991,-1.8621173286,-0.6751205805
C,0,0.5053441028,2.4877999601,0.6011344612
C,0,0.784102332,1.0138176018,0.7750623894
O,0,1.7472970288,0.5136862805,1.2797647883
O,0,-0.2444713753,0.3215896477,0.264398127

C,0,0.6225450124,-1.8067286096,-0.7308253259
O,0,1.3813128215,-2.8855478778,-0.2965206286
O,0,-1.5366686449,-2.9953211524,-0.1953978914
Br,0,1.888600335,3.5953191691,1.3553749735
H,0,-0.0670719337,-1.4921527373,1.3278138224
H,0,-1.4103925491,-1.298535109,-1.4420530196
H,0,0.4284224171,2.7176578285,-0.4570749159
H,0,-0.4316503408,2.7404807469,1.0868088647
H,0,1.0422142653,-1.2095596531,-1.53226739
H,0,1.3695239253,-3.5695214294,-0.9737478253
H,0,-1.538485853,-3.6679421241,-0.8839033839

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.8095934
E (total electronic)+ZPVE = -3069.687494
Internal Thermal Energy = -3069.676440
Enthalpy = -3069.675496
Gibbs Free Energy = -3069.727859

C,0,0.0296458944,-1.3624940235,-0.3031436098
C,0,-1.0057051127,-1.8513975251,-1.101097344
C,0,0.9940462756,-2.0012918305,-1.0852349734
O,0,1.9639892719,-2.7074498047,-0.4996712835
O,0,-2.0810834738,-2.4001653475,-0.5277520531
H,0,0.0088362212,-1.6273166089,0.7449711398
H,0,-1.0300056825,-1.695820276,-2.1697572906
H,0,1.0585296058,-1.8470544253,-2.1526537704
H,0,2.492446311,-3.173942739,-1.1570460389
H,0,-2.6608098749,-2.7910914726,-1.1910110949
C,0,0.8786468988,2.3672559053,0.9287810511
C,0,0.91525824,0.8439728392,0.8187608673
O,0,1.640945101,0.1414777764,1.50338235
O,0,0.0867380251,0.4418141681,-0.0806300014
Br,0,2.1003934412,3.0968746341,2.2469338725
H,0,1.1407600279,2.8080090061,-0.0269836864
H,0,-0.11915017,2.6885977237,1.2075628657

diOHCPr-Dichloroacetate

E (total electronic) = -1415.425155
E (total electronic)+ZPVE = -1415.309486
Internal Thermal Energy = -1415.297656
Enthalpy = -1415.296712
Gibbs Free Energy = -1415.350260

C,0,1.6515972152,-0.314493629,-0.4779270603
C,0,2.743024867,0.6868865647,-0.5357707692
C,0,-1.9603708346,0.2080804102,-0.4884338176
C,0,-0.6453358154,-0.5040430151,-0.1837171819
O,0,-0.5309710879,-1.4757407131,0.5012017223
O,0,0.3513595921,0.1505975667,-0.7759368665
C,0,2.2969743481,0.1103316794,0.7941059104
O,0,3.0604118868,-0.8584471759,1.4298992003
O,0,3.9236198498,0.2566682299,-1.1255664461
Cl,0,-2.0776425823,1.5799076017,0.6418180747
Cl,0,-3.3290550198,-0.8833944421,-0.3192411494
H,0,1.8705874995,-1.314663462,-0.8254085328
H,0,2.4530608583,1.714374856,-0.7219004686
H,0,-1.9597793836,0.6139299628,-1.492056435
H,0,1.7309258548,0.780583419,1.4315886821
H,0,3.8219902053,-0.4370644153,1.8412967524
H,0,4.6654365467,0.6845165623,-0.6859086148

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3775868
E (total electronic)+ZPVE = -1415.264108
Internal Thermal Energy = -1415.252226
Enthalpy = -1415.251281
Gibbs Free Energy = -1415.305569

C,0,-0.5300563501,-1.4312920605,-0.606475303
C,0,0.2446884225,-1.9909910435,-1.625930761
C,0,0.4520837332,-1.8004715502,0.3187887679
O,0,0.1023193333,-2.4695810792,1.4217347115
O,0,-0.3192850604,-2.83438741,-2.5014502623
H,0,-1.5119949762,-1.8583952595,-0.4556942225
H,0,1.2504033578,-1.652971491,-1.8274573511
H,0,1.4699577227,-1.4467452997,0.2418494951
H,0,0.8827502304,-2.7453213952,1.9149378869
H,0,0.3473401363,-3.2234894385,-3.0783925102
C,0,-0.6799367285,2.4996082092,-0.1898176696
C,0,-0.8210009115,1.0155864737,0.2099070608
O,0,-0.6798491816,0.6628710585,1.3655477174
O,0,-1.034321665,0.2786563988,-0.8153026348
Cl,0,-1.1628934565,3.595016055,1.110624262
Cl,0,1.0306896118,2.7606609041,-0.6348903785
H,0,-1.2737432183,2.7315789282,-1.0637218087

diOHCPr-Trifluoroacetate

E (total electronic) = -793.9808697
E (total electronic) + ZPVE = -793.870283
Internal Thermal Energy = -793.858391
Enthalpy = -793.857447
Gibbs Free Energy = -793.910458

C,0,-0.7805310442,-0.2132856079,-0.4409354197
C,0,-1.9574248747,-0.7930708024,0.246779283
C,0,2.8073331896,-0.6478935483,0.1893775149
C,0,1.5137897405,0.0652224876,-0.2592036325
O,0,1.5007140104,1.179794179,-0.6815095103
O,0,0.4849280104,-0.7472175287,-0.0952642242
C,0,-1.5109596221,0.6247063468,0.5490654878
O,0,-2.1989249362,1.7059938892,0.0185711147
O,0,-3.0654381898,-1.0251251581,-0.5553212905
F,0,3.8536824289,0.143689952,0.0179514402
F,0,2.9989468711,-1.7621009837,-0.5144927332
F,0,2.7335562509,-0.9797680046,1.4774822256
H,0,-0.8878541602,0.0545627748,-1.4827941577
H,0,-1.7581361984,-1.5205048918,1.0249785901
H,0,-1.0389717855,0.7724083428,1.5137373304
H,0,-3.0169869108,1.8297249001,0.5110037573
H,0,-3.86233678,-0.8926713468,-0.0317087759

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.9373617

E (total electronic) + ZPVE = -793.828863
Internal Thermal Energy = -793.816949
Enthalpy = -793.816005
Gibbs Free Energy = -793.870219

C,0,-1.1065284814,-0.5239705073,-0.3424466164
C,0,-2.2723166308,-1.1604525253,0.0925767382
C,0,-1.5083641934,0.6181898385,0.358523591
O,0,-1.510744811,1.8063724113,-0.2576942133
O,0,-3.051764356,-1.7906651641,-0.7965241385
H,0,-0.9875769129,-0.4094980164,-1.4114452009
H,0,-2.4937403867,-1.2943371039,1.1408853679
H,0,-1.6758175544,0.6033388608,1.4252745996
H,0,-1.9068122758,2.4806904944,0.3054791285
H,0,-3.8710499226,-2.0838670132,-0.382485879
C,0,2.7991207724,-1.3187081506,0.1052708572
C,0,1.4726366308,-0.6381239071,-0.3307010344
O,0,1.5193036631,0.4282938984,-0.9084089367
O,0,0.4574800085,-1.3311374644,0.0084715786
F,0,2.9054189829,-2.5461928901,-0.4151593515
F,0,3.8657964838,-0.6239083268,-0.2791076351
F,0,2.8533009838,-1.4420534343,1.4368191446

diOHCPr-Trichloroacetate

E (total electronic) = -1875.0189808
E (total electronic)+ZPVE = -1874.913772
Internal Thermal Energy = -1874.900696
Enthalpy = -1874.899752
Gibbs Free Energy = -1874.957293

C,0,-0.929065874,-0.039339509,-0.6610902597
C,0,-2.1030108927,-0.6330830848,0.020253745
C,0,2.6648858342,-0.4716888893,-0.0020788075
C,0,1.3653098127,0.2265118106,-0.4747975869
O,0,1.3298913339,1.3475823763,-0.8784322997
O,0,0.3330107742,-0.5919501596,-0.3409068972
C,0,-1.6443993967,0.7722173697,0.3612115646
O,0,-2.3319641207,1.8735914105,-0.1272997964
O,0,-3.2211955031,-0.8330647148,-0.7768077177
Cl,0,4.0505301142,0.5672948855,-0.3070770217
Cl,0,2.8622068698,-2.0053550821,-0.8660550653
Cl,0,2.5063234136,-0.7683044877,1.7418248104
H,0,-1.0455227421,0.2608231317,-1.693196396
H,0,-1.9008883493,-1.3856717919,0.7734216294
H,0,-1.1604707259,0.8872179443,1.3248082565
H,0,-3.143589091,1.9867959784,0.3780869263
H,0,-4.0115404571,-0.7169691878,-0.2396420841

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1874.9746512
E (total electronic)+ZPVE = -1874.871708
Internal Thermal Energy = -1874.858524
Enthalpy =- 1874.857580
Gibbs Free Energy = -1874.916049

C,0,2.2976606599,0.0883034793,-0.2227857056
C,0,3.2869142843,0.9217122156,0.3059639115
C,0,2.8422323004,-0.9755400572,0.5046436307
O,0,3.1111821884,-2.1319539133,-0.112693242
O,0,4.0020495918,1.7007304399,-0.516278252
H,0,2.2849910185,-0.0270006955,-1.2981425375
H,0,3.4003275188,1.073072648,1.3690500606
H,0,2.9223905836,-0.9485011109,1.5814177301
H,0,3.5771235191,-2.7330788106,0.4791473741
H,0,4.7184005042,2.1327929088,-0.0381196021
C,0,-1.7214762411,0.0802081322,0.0137583323
C,0,-0.2465833673,-0.2800948327,-0.3987649381
O,0,-0.0359521562,-1.3121084367,-0.998810606
O,0,0.5910545573,0.590222309,0.0066407203
Cl,0,-2.0903700891,1.7599697394,-0.4215670233
Cl,0,-2.8891143885,-0.9906590535,-0.7658964724
Cl,0,-1.835347454,-0.1171082218,1.7806885094

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.605137
E (total electronic)+ZPVE = -1269.469115
Internal Thermal Energy = -1269.451810
Enthalpy = -1269.450866
Gibbs Free Energy = -1269.516209

C,0,-2.302391221,-0.5245992084,0.4268599733
C,0,-3.1075233028,0.6969010011,0.6557739105
C,0,-2.7973017627,0.2335747986,-0.7549783238
O,0,-3.7629621132,-0.4182753485,-1.5075523293
O,0,-4.3650498473,0.4951608155,1.2047771576
C,0,1.3416675655,-1.0515931455,0.5539773031
F,0,1.3944273233,-0.6850159961,1.8418647229
C,0,-0.1188183991,-1.2283565934,0.0813793958
O,0,-0.402054557,-1.9638498271,-0.8135279135
O,0,-0.9320533053,-0.4625741016,0.7848995555
F,0,1.9750424929,-2.2256786394,0.4185733618
C,0,2.1499577062,-0.0238709929,-0.2768728117
C,0,1.5396643219,1.3909270706,-0.3590175613
F,0,2.2678152106,-0.4873019276,-1.5279130554
F,0,3.3683409278,0.080050397,0.2670569592
F,0,0.3875889562,1.3391597832,-1.0235947712
F,0,2.3695118237,2.1912783077,-1.007873921
F,0,1.3177540586,1.8824230857,0.8500939317
H,0,-2.770075712,-1.4797632201,0.6210875653
H,0,-2.5675663597,1.5786091535,0.9821009707
H,0,-2.0804181732,0.8353429028,-1.3002000098
H,0,-4.3941131442,0.2300038699,-1.8369498077
H,0,-4.9642914891,1.168840815,0.8672566976

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.5633699
E (total electronic)+ZPVE = -1269.429418
Internal Thermal Energy = -1269.412185
Enthalpy = -1269.411240
Gibbs Free Energy = -1269.476205

C,0,-0.76175928,-2.1149618614,-0.0204929161
C,0,-1.5742779824,-2.5355916906,-1.0794052657

C,0,0.2590474977,-2.8924357495,-0.5815757878
O,0,0.9100522468,-3.7742807821,0.1880318365
O,0,-2.7879222977,-3.0453754005,-0.8193675442
H,0,-1.0824635805,-2.4004785126,0.9720169549
H,0,-1.3329266159,-2.3089574466,-2.1073706016
H,0,0.6515027056,-2.6977811578,-1.5685558693
H,0,1.5171137473,-4.3040418507,-0.3403321111
H,0,-3.191919511,-3.3872314211,-1.6245751599
C,0,0.7683181557,1.5484832978,0.068363527
F,0,-0.3652234392,2.2257490523,0.3261874566
C,0,0.6103225759,0.032036221,0.3753318094
O,0,1.6135608422,-0.6009688516,0.6336414335
O,0,-0.5940844717,-0.3678602677,0.260249
F,0,1.7434947777,2.0730411915,0.8343319046
C,0,1.1665506021,1.8428666561,-1.396322001
C,0,0.2695224704,1.1945286275,-2.4717314581
F,0,2.4173810776,1.4066578406,-1.6047812378
F,0,1.1389378306,3.1708847712,-1.5886587266
F,0,0.4068494538,-0.1291634961,-2.4395875541
F,0,0.6396524701,1.624775662,-3.6699934619
F,0,-1.0040512751,1.5023281684,-2.2800512272

---

diOHCPr-Propanoate

E (total electronic) = -535.5308819
E (total electronic) + ZPVE = -535.368796
Internal Thermal Energy = -535.357530
Enthalpy = -535.356586
Gibbs Free Energy = -535.406636

C,0,-1.3010005831,-0.3099829298,-0.4484354866
C,0,-2.5026394363,-0.8833257675,0.2049165626
C,0,2.277957105,-0.7556202826,0.1646406084
C,0,1.013443972,-0.0663146404,-0.2619206805
O,0,0.9297799295,1.0481908063,-0.7066081171
O,0,-0.0598450816,-0.8647614301,-0.0916772746
C,0,-2.0456668192,0.5241498331,0.534817665
O,0,-2.7187951544,1.62013591,0.0088848773
O,0,-3.6025030991,-1.0876600862,-0.6204063834
C,0,3.5109224953,0.1085697814,-0.0254148915
H,0,-1.400522081,-0.0213159734,-1.4862800649
H,0,-2.3334577961,-1.6261176786,0.9757141207
H,0,2.1478585986,-1.0497337147,1.2074612513
H,0,2.3454549587,-1.68542337,-0.4023405845
H,0,-1.5924465082,0.657353401,1.5104804413
H,0,-3.5427234615,1.7422270504,0.4912199574
H,0,-4.4058834645,-0.9437783551,-0.1103508484
H,0,4.3996752487,-0.4316423631,0.2936222683
H,0,3.6328400607,0.3851749466,-1.071105254
H,0,3.4366251166,1.0243978626,0.5581058333

TS–diOHCPr-Propanoate

E (total electronic) = -535.4729963
E (total electronic) + ZPVE = -535.313216
Internal Thermal Energy = -535.301808
Enthalpy = -535.300864
Gibbs Free Energy = -535.353188

C,0,-1.91774063,-0.3755364028,-0.1075530588
C,0,-2.9512510071,-1.2430768122,0.2417190384
C,0,-2.5193055721,0.7372475918,0.4787791879
O,0,-2.54696646,1.9001751793,-0.1717089026
O,0,-3.4183781671,-2.1141894308,-0.6543926144
H,0,-1.6632704668,-0.2955666841,-1.1549177783
H,0,-3.3270932854,-1.3113048367,1.2524755489
H,0,-2.87889794,0.7232551839,1.497895378
H,0,-3.0754931522,2.5493134657,0.3063193698
H,0,-4.1923633544,-2.5776171064,-0.3147247532
C,0,2.1169701355,-0.8232267308,0.280545247
C,0,0.7456330975,-0.3252317566,-0.1556951361
O,0,0.6259236579,0.5423601074,-1.0198945037
O,0,-0.2387791335,-0.8905819886,0.4583370951
C,0,3.2773256026,-0.1670268517,-0.4464394474
H,0,2.186715894,-0.6634519893,1.3579892918
H,0,2.1248149704,-1.9053935534,0.1396274532
H,0,4.2267712061,-0.5603482987,-0.0853532633
H,0,3.2175515982,-0.3486347674,-1.5183777664
H,0,3.2724970062,0.9108916813,-0.292925386

diOHCPr-Butanoate

E (total electronic) = -574.8379903
E (total electronic) + ZPVE = -574.647126
Internal Thermal Energy = -574.634670
Enthalpy = -574.633726
Gibbs Free Energy = -574.686812

C,0,1.2173656959,-0.2547781506,0.3019676341
C,0,2.475745221,-0.8354257098,-0.2270170897
C,0,2.0734874489,0.5821773761,-0.5829235697
O,0,2.7005490485,1.6613428429,0.0278098117
O,0,3.4794645564,-1.063706973,0.7073189323
C,0,-2.2588956453,-0.6042027627,-0.7873515625
C,0,-1.0534426254,0.0351738548,-0.1553603439
O,0,-1.0026284635,1.1408350613,0.3156103168
O,0,0.0154626957,-0.7862696708,-0.1971872719
C,0,-3.5592058448,0.1143322584,-0.4599790683
C,0,-3.9633058132,-0.0480764406,1.0003173856
H,0,1.2067230898,0.0175448143,1.3487902043
H,0,2.3817744022,-1.5658973882,-1.0220644747
H,0,1.7286464906,0.7347446203,-1.5992426948
H,0,3.5728135413,1.7781619581,-0.3621351686
H,0,4.3332861828,-0.9063908833,0.2917747709
H,0,-2.290392342,-1.6502189108,-0.4795515598
H,0,-2.0677319364,-0.6075219818,-1.8633587802
H,0,-3.4534053743,1.1716188956,-0.7041374953
H,0,-4.3415598096,-0.2845321909,-1.1055933002
H,0,-4.897625925,0.4712164087,1.208893342
H,0,-4.1016189957,-1.1019236026,1.2458832227
H,0,-3.1986455979,0.3560905743,1.663585759

TS–diOHCPr-Butanoate

E (total electronic) = -574.7801415
E (total electronic) + ZPVE = -574.591564

Internal Thermal Energy = -574.579024
Enthalpy = -574.578080
Gibbs Free Energy = -574.632629

C,0,2.3318149762,0.0454468797,1.0192264846
C,0,1.01656986,0.2269806337,0.269028708
O,0,0.9569447613,0.9214221808,-0.7453090931
O,0,0.0084338294,-0.3683473148,0.8106723765
C,0,3.5700549989,0.2563002261,0.160593525
C,0,3.7340410364,-0.8341325321,-0.8912583407
H,0,2.3071648662,0.7636961313,1.8431267423
H,0,2.3352725867,-0.9459135687,1.4738332775
H,0,3.5051038395,1.2307832348,-0.3235056274
H,0,4.4484056805,0.2778423528,0.8076363465
H,0,2.8685630485,-0.8609473266,-1.5538399879
H,0,3.8279308628,-1.8135357048,-0.4190687551
H,0,4.6213541351,-0.6697181675,-1.5019461305
C,0,-1.6059433787,-0.1131214705,-0.045215304
C,0,-2.6075543554,-1.0205347087,0.2958178334
C,0,-2.3712476564,1.0058978937,0.2808392296
O,0,-2.396373805,2.0575135578,-0.5376882099
O,0,-2.8734711142,-2.0508512476,-0.5090559724
H,0,-1.2104321535,-0.1566210872,-1.050020973
H,0,-3.1164554228,-0.9835761963,1.2483492953
H,0,-2.8709733983,1.0999620695,1.2343890334
H,0,-3.0366228473,2.7125424673,-0.2372886476
H,0,-3.6502631262,-2.5340203071,-0.2050413319

diOHCPr-Phenylacetate

E (total electronic) = -727.2595022
E (total electronic) + ZPVE = -727.044000
Internal Thermal Energy = -727.029710
Enthalpy = -727.028765
Gibbs Free Energy = -727.088035

C,0,-2.4870901916,-0.3566356836,-0.2287155715
C,0,-3.7716131634,-0.4437270826,0.5075580964
C,0,0.9649575605,-0.9162180131,0.8402492359
C,0,-0.1694924429,-0.3226812203,0.0391240575
O,0,-0.0754323416,0.5000711756,-0.8305716354
O,0,-1.3454866107,-0.848059584,0.4300992835
C,0,-3.1246228339,0.9020857288,0.2459943029
O,0,-3.623108203,1.73611286,-0.7469542108
O,0,-4.872349826,-0.8477967663,-0.2385845023
H,0,-2.5198438746,-0.5341075234,-1.2952761677
H,0,-3.7258280269,-0.7976735181,1.5308208539
H,0,0.7679403591,-0.684391346,1.8879978004
H,0,0.8921771738,-2.0002238867,0.7437647216
H,0,-2.6767300807,1.3866944665,1.1059848307
H,0,-4.431550342,2.151585752,-0.4302252549
H,0,-5.6558874904,-0.3985515951,0.0941822494
C,0,2.3149930625,-0.4172878803,0.4129296578
C,0,2.9965267418,-1.0390893792,-0.628974325
C,0,2.8942792351,0.6835504618,1.0354483856
C,0,4.2348199475,-0.5688860034,-1.0434985722
H,0,2.5541936102,-1.8988435903,-1.1171473476
C,0,4.1334345487,1.1568914959,0.6240987109
H,0,2.3726597068,1.1718978509,1.849323032
C,0,4.8062829554,0.5316692532,-0.417317071
H,0,4.7548223647,-1.0628303952,-1.8530152698
H,0,4.5738519745,2.0120670896,1.1185351059
H,0,5.7723661874,0.8975383331,-0.7370813961

TS–diOHCPr-Phenylacetate

E (total electronic) = -727.2035627
E (total electronic) + ZPVE = -726.990290
Internal Thermal Energy = -726.975978
Enthalpy = -726.975034
Gibbs Free Energy = -727.035875

C,0,-2.846030559,-0.1060734962,-0.096521803
C,0,-4.0473406386,-0.6230475736,0.3866987251
C,0,-3.3109598738,1.2089949173,-0.0825414116
O,0,-3.0929512022,2.003960278,-1.1302836405
O,0,-4.5792591414,-1.7088889036,-0.1787946012
C,0,0.9873817268,-0.7426658004,1.1138645695
C,0,-0.2302795449,-0.2930822186,0.2968193645
O,0,-0.108404427,0.2484952114,-0.7975949297
O,0,-1.350861756,-0.5529018409,0.8762711217
C,0,2.3094898866,-0.3566275126,0.5208270782
C,0,2.9446401367,-1.1816252078,-0.4037407657
C,0,2.9165217382,0.8481218423,0.8653370463
C,0,4.1548847905,-0.8115067308,-0.9747178706
C,0,4.1270343415,1.2238885248,0.2978020393
C,0,4.750033118,0.3945008626,-0.6257993485
H,0,-2.4868177704,-0.482302267,-1.0440513324
H,0,-4.5191702299,-0.2397528338,1.2797791633
H,0,-3.7545373564,1.6496679605,0.7989039384
H,0,-3.5528502517,2.84472034,-1.0261725195
H,0,-5.4533229095,-1.8918838799,0.1839554564
H,0,0.8721767107,-0.3266210594,2.1148992349
H,0,0.9086773097,-1.8262960304,1.2150106742
H,0,2.4849206803,-2.1234672159,-0.6779928275
H,0,2.4354362108,1.4973778471,1.5868909718
H,0,4.6351344088,-1.4655104121,-1.6902282643
H,0,4.5851019865,2.1628326016,0.5786466524
H,0,5.6939961881,0.6834987652,-1.0674160747

diOHCPr-Propenoate

E (total electronic) = -534.3003972
E (total electronic) + ZPVE = -534.161411
Internal Thermal Energy = -534.150872
Enthalpy = -534.149928
Gibbs Free Energy = -534.198199

C,0,-0.3636898724,-0.7162792189,-0.0239164885
C,0,-0.0395084967,-1.5876191125,-1.1792006185
C,0,-0.0308327558,1.399258547,0.8981184458
O,0,0.003545485,0.9176156651,2.001603315
O,0,-0.2233339697,0.6691613497,-0.2165012852
C,0,0.8510195523,-1.5750188443,0.047743688
O,0,0.7971868333,-2.6188824346,0.9627255227
O,0,-0.9105770269,-2.6474461025,-1.4017635171
C,0,0.1197501536,2.8351121628,0.5697102932
C,0,0.3055403248,3.7273459539,1.5305467383

H,0,-1.1953316948,-1.016386441,0.599298358
H,0,0.3659498116,-1.1026316182,-2.0594897398
H,0,1.8094740529,-1.0824254199,-0.0693277315
H,0,1.2578400208,-3.380379662,0.5960808396
H,0,-0.4108735969,-3.3944772532,-1.7460783216
H,0,0.0698014654,3.1049336032,-0.4755366508
H,0,0.3487732644,3.4187006377,2.5670550154
H,0,0.4176574489,4.7786821878,1.3070871372

TS–diOHCPr-Propenoate

E (total electronic) = -534.2442629
E (total electronic) + ZPVE = -534.107705
Internal Thermal Energy = -534.096951
Enthalpy = -534.096007
Gibbs Free Energy = -534.146392

C,0,-0.9966552964,-1.5492563992,-0.4943688572
C,0,-2.1728783834,-2.2884670109,-0.3751983568
C,0,-1.2262750584,-1.2505894276,-1.837467813
O,0,-0.2393276989,-1.3742150656,-2.7255556302
O,0,-2.1518096524,-3.473280458,0.2400292911
H,0,-0.0678950545,-2.051221728,-0.2622696586
H,0,-3.1339307198,-1.8903465743,-0.6669408826
H,0,-2.154923284,-0.8133318421,-2.1754500932
H,0,-0.5644235086,-1.233613265,-3.6220526571
H,0,-3.0029248735,-3.9184012106,0.1595905327
C,0,0.389675794,0.3159890649,0.7761838944
O,0,1.3391890834,-0.0302537104,0.0747620028
O,0,-0.7972010907,-0.1841049323,0.7185656501
C,0,1.6925858169,2.0144780074,2.0175412655
C,0,0.5388571051,1.3998174139,1.8072124963
H,0,1.7939823599,2.791226536,2.7632501923
H,0,2.5675237752,1.7460952203,1.4392996159
H,0,-0.3497183139,1.6486963819,2.3728000076

diOHCPr-Propynoate

E (total electronic) = -533.0440847
E (total electronic) + ZPVE = -532.929239
Internal Thermal Energy = -532.918837
Enthalpy = -532.917892
Gibbs Free Energy = -532.965837

C,0,-0.2904846276,-1.2462660046,0.3892590168
C,0,-1.3089327338,-2.2151139247,-0.081758537
C,0,0.2844092187,1.0033283996,0.3904153901
O,0,1.4460583806,0.7378631194,0.2433027725
O,0,-0.6967803966,0.1012450187,0.4901878723
C,0,-0.1216303416,-1.861108048,-0.9559497721
O,0,0.9440100343,-2.7417961074,-1.0813328859
O,0,-1.3440305221,-3.4269603387,0.5953700164
C,0,-0.2337815583,2.3549300485,0.4894253062
C,0,-0.6235470865,3.482508166,0.568067613
H,0,0.391196738,-1.5790849693,1.1599548695
H,0,-2.2622519675,-1.8081859507,-0.3981397894
H,0,-0.3385044779,-1.2350614297,-1.8138735625
H,0,0.6922577633,-3.4560750533,-1.6756000715
H,0,-1.5743254616,-4.1249617795,-0.0261662851
H,0,-0.9718889614,4.4873198537,0.6388440469

TS–diOHCPr-Propynoate

E (total electronic) = -532.9946477
E (total electronic) + ZPVE = -532.881967
Internal Thermal Energy = -532.871532
Enthalpy = -532.870587
Gibbs Free Energy = -532.919613

C,0,-1.7965862092,-0.482567416,-0.3176455107
C,0,-2.912564241,-1.2450987896,0.0325310638
C,0,-2.3594126327,0.6477859107,0.2804480001
O,0,-2.3835840783,1.8077645989,-0.3823416887
O,0,-3.4977135691,-2.0223955507,-0.8855160596
H,0,-1.5691838405,-0.4042632064,-1.3718572055
H,0,-3.2476829129,-1.3344514501,1.0553704193
H,0,-2.6624528349,0.6537635767,1.3171842476
H,0,-2.8887434192,2.4691973613,0.1037228715
H,0,-4.3131120935,-2.4038208821,-0.5412315564
C,0,0.8143020667,-0.4334896312,-0.1907559008
O,0,0.7831477663,0.546184775,-0.9229062703
O,0,-0.188287128,-1.1136925022,0.2318455275
C,0,2.1126966616,-0.9358417811,0.2941981642
C,0,3.1742735328,-1.335301967,0.6798778277
H,0,4.1184059318,-1.6899860462,1.0224100703

diOHCPr-Difluoroacetate

E (total electronic) = -694.7181827
E (total electronic) + ZPVE = -694.599050
Internal Thermal Energy = -694.587874
Enthalpy = -694.586930
Gibbs Free Energy = -694.638130

C,0,-1.096061954,-0.103280816,-0.4680558394
C,0,-2.1873899459,-0.9059020083,0.1331971187
C,0,2.5432846024,-0.4120891882,-0.1947468753
C,0,1.1907236938,0.2894088837,-0.3591164195
O,0,1.0616960902,1.4675410675,-0.5096241466
O,0,0.215558725,-0.6116987941,-0.3337693903
C,0,-1.7966178908,0.431936382,0.7310359978
O,0,-2.5812747493,1.5552602189,0.5114082109
O,0,-3.3394783264,-1.02317812,-0.6323604448
F,0,2.5328029329,-1.1268779592,0.9563052389
F,0,3.5101646601,0.5171695491,-0.095698683
H,0,-1.2988847152,0.3894094664,-1.4090280729
H,0,-1.8938264925,-1.7779049375,0.7057951354
H,0,2.7616505978,-1.080299381,-1.0264413615
H,0,-1.2628530557,0.3877179238,1.6734587863
H,0,-3.3564205479,1.5124911661,1.0808081597
H,0,-4.1018806244,-1.0540104531,-0.0454364144

TS–diOHCPr-Difluoroacetate

E (total electronic) = -694.6707193
E (total electronic) +ZPVE = -694.553834
Internal Thermal Energy = -694.542595
Enthalpy = -694.541651

Gibbs Free Energy = -694.594151

C,0,-1.4549422548,-0.0890837502,-0.1374377132
C,0,-2.5035697249,-0.9316028491,0.2379857137
C,0,-1.9649769336,0.9211586789,0.6824462428
O,0,-2.1071954297,2.1594551171,0.199376588
O,0,-3.1931687485,-1.5885578539,-0.7021020252
C,0,2.5460711869,-0.5219207172,-0.0976639127
C,0,1.1391754061,0.0581001783,-0.3426558097
O,0,1.0085117351,1.1231089028,-0.9192392192
O,0,0.2237479651,-0.7156192964,0.1058736133
F,0,2.720674909,-0.7324591901,1.2361693417
F,0,3.4994550182,0.3544698009,-0.4862627463
H,0,-1.3711667447,0.1460753079,-1.1897494289
H,0,-2.6966048444,-1.1814207576,1.2708222494
H,0,-2.124182915,0.7724328635,1.7402586512
H,0,-2.5602803886,2.7237190332,0.8359370779
H,0,-3.9522115365,-2.0396039209,-0.3159251867
H,0,2.6982725002,-1.4655652435,-0.6195428423

diOHCPr-Dibromoacetate

E (total electronic) = -5643.4941564
E (total electronic)+ZPVE = -5643.379620
Internal Thermal Energy = -5643.367384
Enthalpy = -5643.366440
Gibbs Free Energy = -5643.421740

C,0,2.3883696977,-0.6138257901,-0.334926463
C,0,3.4990934805,0.2616995732,-0.7787920077
C,0,-1.2069890071,-0.0572554839,-0.5573165147
C,0,0.0890222837,-0.6217411611,0.0028012736
O,0,0.1932595827,-1.2449093221,1.0173953058
O,0,1.097255307,-0.2806164227,-0.8003711396
C,0,3.04397983,0.2692084905,0.6678802784
O,0,3.7892482328,-0.3812254061,1.6410632853
O,0,4.6704203945,-0.3890939201,-1.1415073221
Br,0,-1.355079292,1.756585539,0.1197445533
Br,0,-2.7147115388,-1.1413364775,-0.0757068133
H,0,2.5875405918,-1.6735562746,-0.2549586542
H,0,3.2292268194,1.136066621,-1.359451486
H,0,-1.1722461965,0.0160878351,-1.6355132994
H,0,2.4918496218,1.147896105,0.9831691012
H,0,4.5641040396,0.1505433366,1.8496248889
H,0,5.4205711531,0.1695597578,-0.9137549867

TS–diOHCPr-Dibromoacetate

E (total electronic) = -5643.4464296
E (total electronic)+ZPVE = -5643.334215
Internal Thermal Energy = -5643.321887
Enthalpy = -5643.320942
Gibbs Free Energy = -5643.378144

C,0,2.6591082255,-0.4677404534,-0.4707522779
C,0,3.410181003,0.7046120701,-0.3389145291
C,0,2.8399577579,-0.7067594746,0.8966019756
O,0,3.2798806066,-1.9016436039,1.3057757462
O,0,4.4136157413,0.9502358378,-1.1932705575
H,0,3.0526966993,-1.2185604362,-1.1419686693
H,0,3.1121455359,1.4989836725,0.3297738057
H,0,2.5033496668,-0.0068253103,1.647286772
H,0,3.4513982342,-1.894520663,2.253925464
H,0,4.9050683499,1.7339557466,-0.9237606295
C,0,-1.1868020212,0.1219019872,-0.6175421489
C,0,0.0913959042,-0.7068619202,-0.4049235849
O,0,0.1538024297,-1.5662364622,0.4537010203
O,0,1.0329987399,-0.3126187835,-1.1823241864
Br,0,-2.7934714304,-0.873719286,-0.2487630551
Br,0,-1.0263871909,1.6840654508,0.5345526784
H,0,-1.2579572515,0.4976776282,-1.6283358237

diOHCPr-Tribromoacetate

E (total electronic) = -8217.1199267
E (total electronic)+ZPVE = -8217.016585
Internal Thermal Energy = -8217.002653
Enthalpy = -8217.001709
Gibbs Free Energy = -8217.061666

C,0,-0.9910876594,0.00757239,-0.7507080934
C,0,-2.1597484917,-0.5720885515,-0.0469641522
C,0,2.6003517565,-0.405820351,-0.0704599804
C,0,1.3018387265,0.2823309121,-0.5429404878
O,0,1.2516016391,1.4112980967,-0.925682366
O,0,0.2714481328,-0.547479159,-0.4404047162
C,0,-1.6881255656,0.8338820902,0.2716389759
O,0,-2.3758155856,1.9343524774,-0.2188463433
O,0,-3.2904660312,-0.7739712421,-0.8258653321
Br,0,2.3909556292,-0.7825395656,1.8244457352
Br,0,2.8536825616,-2.0490391951,-1.0667522418
Br,0,4.1059105877,0.7633829266,-0.3434890561
H,0,-1.1201954993,0.2969032254,-1.7844573291
H,0,-1.9517113424,-1.3177142948,0.7115575557
H,0,-1.1897337994,0.9562962856,1.2270981102
H,0,-3.1745288948,2.0631097533,0.3029444343
H,0,-4.0724911641,-0.6364257984,-0.2815337128

TS–diOHCPr-Tribromoacetate

E (total electronic) = -8217.0752858
E (total electronic)+ZPVE = -8216.974081
Internal Thermal Energy = -8216.960176
Enthalpy = -8216.959232
Gibbs Free Energy = -8217.019921

C,0,-2.9127648679,-0.0399706924,-0.6330578564
C,0,-3.6363983697,-0.7754871627,0.3124149377
C,0,-3.2759319902,1.1165585288,0.0689936128
O,0,-3.8272365053,2.1432761144,-0.5905426738
O,0,-4.5382837284,-1.6786535988,-0.1004258775
H,0,-3.2557362446,-0.1033606338,-1.656580625
H,0,-3.3772440593,-0.7640634747,1.3608937368
H,0,-2.9884482109,1.2711742095,1.0987600316
H,0,-4.116374041,2.825632145,0.0251897512
H,0,-5.0306324947,-2.0336037748,0.6478354344
C,0,0.9571090534,0.0141645611,-0.0742370795
C,0,-0.407917768,0.4851452106,-0.6831294317

O,0,-0.6130935583,1.6725923306,-0.8213782733
O,0,-1.215969666,-0.4814017466,-0.8887718943
Br,0,1.5760664816,-1.6270947402,-0.8953182178
Br,0,2.3179186942,1.3733322353,-0.2540603338
Br,0,0.5807293152,-0.2909028401,1.8171609084

diOHCPr-Pentafluoropropanoate

E (total electronic) = -1031.794201
E (total electronic)+ZPVE = -1031.671059
Internal Thermal Energy = -1031.656334
Enthalpy = -1031.655389
Gibbs Free Energy = -1031.715650

C,0,-1.3224045578,0.2067936205,-0.4929296977
C,0,-2.231216167,-0.9613144124,-0.4263144095
C,0,2.3523764717,0.3593931253,-0.4926257963
C,0,0.8992254026,0.8171117803,-0.2449969067
O,0,0.6456248203,1.8270360875,0.3363768867
O,0,0.047306919,-0.0664037785,-0.7322194188
C,0,-1.9139701195,-0.1600873605,0.8223982075
O,0,-2.8351430004,0.7424488501,1.3320443879
O,0,-3.4506783521,-0.8067127015,-1.0694027121
C,0,2.8416845611,-0.6318609657,0.5838977788
F,0,4.1086455325,-0.9505562742,0.3610241399
F,0,2.741481215,-0.0766750352,1.7858545257
F,0,2.1098497246,-1.7382738337,0.5591987519
F,0,2.4760157679,-0.2378468683,-1.6870148277
F,0,3.1587089045,1.4264600082,-0.4556054895
H,0,-1.6922194995,1.1064342691,-0.9645387619
H,0,-1.7716721947,-1.9413192175,-0.4809827255
H,0,-1.2600972081,-0.6464007229,1.5378505845
H,0,-3.5231315095,0.258087882,1.8001041889
H,0,-4.1240387105,-1.2947014526,-0.5843257059

TS–diOHCPr-Pentafluoropropanoate

E (total electronic) = -1031.751271
E (total electronic)+ZPVE = -1031.630256
Internal Thermal Energy = -1031.615555
Enthalpy = -1031.614610
Gibbs Free Energy = -1031.675618

C,0,0.2567901118,-2.0008109221,-0.3561039794
C,0,0.0145017023,-2.7921357463,-1.4826031683
C,0,1.5388608886,-2.5574739054,-0.2897501998
O,0,1.9797570131,-3.0654101069,0.8675284945
O,0,-1.0999825552,-3.5341661318,-1.5392224499
H,0,-0.3808608326,-2.1710295939,0.500800976
H,0,0.6139686984,-2.713178504,-2.3772301602
H,0,2.2465634417,-2.459212958,-1.0994567262
H,0,2.8293763937,-3.5032587876,0.7449605109
H,0,-1.0831766678,-4.1149844404,-2.3078777489
C,0,0.3969473683,1.9678064547,0.2503900776
C,0,0.4304530998,0.4297506828,0.4867953439
O,0,0.8631172133,0.0268172835,1.5475434313
O,0,0.0123260443,-0.2310243439,-0.5186178435
C,0,1.6673727221,2.4839262199,-0.4488396001
F,0,0.3016388205,2.6181561814,1.4234714433
F,0,-0.6522908101,2.3286121732,-0.5124926389
F,0,1.789824397,1.9444729486,-1.6566640654
F,0,2.7441999071,2.1736190837,0.2664825729
F,0,1.6166570435,3.8058454125,-0.5821692698

diOHCPr-Pentachloropropanoate

E (total electronic) = -2833.5311802
E (total electronic)+ZPVE = -2833.417098
Internal Thermal Energy = -2833.400501
Enthalpy = -2833.399557
Gibbs Free Energy = -2833.463755

C,0,-1.6324986573,-0.0411201436,-0.4764961181
C,0,-2.791838313,-0.649775912,0.2176732517
C,0,1.9795308119,-0.4596631751,0.0807822324
C,0,0.6617643837,0.2436901381,-0.3314496054
O,0,0.5949159195,1.369788561,-0.7195237535
O,0,-0.361320667,-0.5862084447,-0.1836143178
C,0,-2.3370667596,0.7551453747,0.5646198489
O,0,-3.039340011,1.8573505653,0.0994314738
O,0,-3.9203086472,-0.8500004132,-0.5650207156
C,0,3.2363957851,0.4546250744,-0.095463239
Cl,0,1.8214305834,-0.9261970445,1.7870834492
Cl,0,2.1600283484,-1.9123910233,-0.9234183486
Cl,0,4.6946148731,-0.4296320473,0.3959485069
Cl,0,3.4105910404,0.9297861877,-1.7933014099
Cl,0,3.0916337717,1.9021034077,0.9156212352
H,0,-1.7695810584,0.2677824727,-1.5035084665
H,0,-2.5737978538,-1.4081986389,0.9604607006
H,0,-1.8381221047,0.8628244267,1.5213064223
H,0,-3.8339982474,1.9696745526,0.6311408989
H,0,-4.7042461978,-0.7253299187,-0.0204450454

TS–diOHCPr-Pentachloropropanoate

E (total electronic) = -2833.4862155
E (total electronic)+ZPVE = -2833.374253
Internal Thermal Energy = -2833.357654
Enthalpy = -2833.356710
Gibbs Free Energy = -2833.422044

C,0,0.0316560214,-1.9885512926,-0.5768166172
C,0,0.2499097277,-2.9654299931,-1.5518711131
C,0,0.9594288583,-2.6357628418,0.2460442008
O,0,0.6380357454,-2.916790074,1.5141555359
O,0,-0.7978718551,-3.5768467663,-2.1199514295
C,0,0.4934743443,2.0207678115,-0.5429569869
C,0,0.1468496534,0.5464334731,-0.1036619009
O,0,-0.1695284451,0.3170387989,1.0447586315
O,0,0.2587965252,-0.2774802911,-1.0691119749
C,0,0.3365506867,3.0837531765,0.5896838858
Cl,0,-0.5812745001,2.4547430619,-1.8935630268
Cl,0,2.1799776741,2.0269557512,-1.1124953093
Cl,0,1.4268323428,2.7236588115,1.9404601571
Cl,0,-1.3380249717,3.1182672673,1.1718815433
Cl,0,0.7420047704,4.7062591243,-0.0228762677
H,0,-0.9744636732,-1.9072915984,-0.1882274472
H,0,1.2275530494,-3.1445935847,-1.9742158849

H,0,1.9834129036,-2.7899730354,-0.0603045835
H,0,1.3241426524,-3.4516714216,1.9289360133
H,0,-0.5046495096,-4.2983663771,-2.687384426

diOHCPr-Pentabromopropanoate

E (total electronic) = -13403.6977458
E (total electronic)+ZPVE=-13403.586882
Internal Thermal Energy = -13403.568761
Enthalpy = -13403.567817
Gibbs Free Energy = -13403.637793

C,0,3.4537058609,0.0012165081,0.6009700686
C,0,4.6443533615,-0.5095641541,-0.1186290771
C,0,-0.1327338162,-0.4537632441,-0.1011447803
C,0,1.1525467779,0.2196933707,0.4346366872
O,0,1.1788866442,1.2979612726,0.9465570703
O,0,2.2092754776,-0.5582413391,0.2345656583
C,0,4.1483075155,0.9041318381,-0.3567980438
O,0,4.8060683474,1.9858043915,0.2106144349
O,0,5.7659126859,-0.7376293173,0.6665599843
C,0,-1.4226995915,0.3774580984,0.1689644009
Br,0,0.1339589657,-0.6865214946,-2.019092118
Br,0,-0.2696739675,-2.2054435337,0.7407209209
Br,0,-2.9910680046,-0.539003728,-0.5300118749
Br,0,-1.6770032237,0.6346044978,2.0818412959
Br,0,-1.3290009245,2.1219095038,-0.6902571259
H,0,3.5626307244,0.2266126547,1.6527690301
H,0,4.4642175236,-1.2107040544,-0.9251702321
H,0,3.6606453196,1.07495549,-1.3103261176
H,0,5.6026536998,2.1698015581,-0.2976465869
H,0,6.5543036239,-0.5532383185,0.1459244051

TS–diOHCPr-Pentabromopropanoate

E (total electronic) = -13403.6521115
E (total electronic)+ZPVE=-13403.543512
Internal Thermal Energy = -13403.525309
Enthalpy = -13403.524364
Gibbs Free Energy = -13403.595603

C,0,-3.1533049674,0.0141364395,-0.2159178519
C,0,-4.2672952732,-0.7395244191,0.162453288
C,0,-3.6050610443,1.0575489581,0.5985162906
O,0,-3.6815086141,2.2988790499,0.1055869148
O,0,-5.0126050541,-1.3335573367,-0.7783566373
H,0,-3.054073345,0.2389390877,-1.269071586
H,0,-4.4704846347,-0.9835993819,1.1946737555
H,0,-3.7623180212,0.9260355512,1.6588459075
H,0,-4.1052235042,2.8904443068,0.7375643837
H,0,-5.8055785129,-1.7200822166,-0.3907019707
C,0,0.8289342382,-0.5309665404,0.1968301205
C,0,-0.5713957416,0.0540236883,-0.2328520454
O,0,-0.6266072804,1.1486723379,-0.754362821
O,0,-1.5382490133,-0.7275417455,0.0477765756
C,0,2.0485395843,0.3558412316,-0.1842381801
Br,0,3.7286104256,-0.4614836594,0.3817209371
Br,0,1.0029277896,-2.2878557113,-0.6353528855
Br,0,2.1367187028,0.6059918107,-2.114257622
Br,0,1.9443554332,2.1051635129,0.6670655718
Br,0,0.7588623325,-0.7651108335,2.1339601345

diOHCPr-Heptachlorobutanoate

E (total electronic) = -3792.031481
E (total electronic)+ZPVE = -3791.908443
Internal Thermal Energy = -3791.888576
Enthalpy = -3791.887631
Gibbs Free Energy = -3791.958675

C,0,0.26884246,-1.4955848164,-0.2618331839
C,0,0.5010245158,-2.2039578066,-1.5423864685
C,0,1.531441143,-2.2652073444,-0.4306255051
O,0,1.6463056711,-3.3990490992,0.3602093246
O,0,-0.3326653244,-3.2855884193,-1.7888311816
C,0,0.6226939503,2.0596562784,0.6907463937
C,0,0.6267954597,0.507556827,0.8388644619
O,0,0.9028659412,-0.0458372505,1.8585808056
O,0,0.3084392472,-0.0831299404,-0.3018932669
C,0,-0.8309682236,2.7008028015,0.5359734732
C,0,-1.9241090121,2.2634046918,1.6032630307
H,0,-0.4669955486,-1.9080912628,0.415776303
H,0,0.7710502798,-1.5929477482,-2.3958066165
H,0,2.4372626772,-1.6935163937,-0.5981668804
H,0,2.1186839418,-4.0782566724,-0.1320913343
H,0,0.1555926178,-3.9482265195,-2.2881583672
Cl,0,1.4994004892,2.7214184092,2.0777317926
Cl,0,1.5830749794,2.4653741179,-0.7568708417
Cl,0,-2.2581100523,0.5221583226,1.4872862159
Cl,0,-1.4884790234,2.2725594385,-1.0598099754
Cl,0,-3.44444471,3.1261154298,1.2768655254
Cl,0,-0.6568363137,4.4653763159,0.6116130599
Cl,0,-1.4415277854,2.6338044009,3.261311525

TS–diOHCPr-Heptachlorobutanoate

E (total electronic) = -3791.986822
E (total electronic)+ZPVE = -3791.866007
Internal Thermal Energy = -3791.846070
Enthalpy = -3791.845125
Gibbs Free Energy = -3791.916953

C,0,0.7946635912,-1.7663202313,0.602965424
C,0,0.5365721641,-2.9219019887,-0.1393647204
C,0,1.8913720519,-2.411446832,1.183651559
O,0,2.0380754275,-2.3966819173,2.5139070912
O,0,-0.7044275003,-3.4264397558,-0.1624276979
H,0,0.0185539373,-1.4459780168,1.2860879984
H,0,1.264009508,-3.343706694,-0.8167169086
H,0,2.7082096163,-2.7955275628,0.5907393408
H,0,2.7710539302,-2.9620302478,2.7821248471
H,0,-0.7171278451,-4.2781889665,-0.6130259008
C,0,1.0683496781,2.1575877633,-0.3553007315
C,0,1.0265471251,0.7960812322,0.4551105665
O,0,1.0373962265,0.8396149305,1.6666698914
O,0,0.9848062451,-0.2303915543,-0.2974517869
C,0,-0.3222190257,2.5507641959,-1.0235158142

C,0,-1.6069064541,2.5159283092,-0.0875586116
Cl,0,1.6667551944,3.4358049239,0.7216702561
Cl,0,2.2884909756,1.9963611359,-1.6508496446
Cl,0,-1.4484300414,3.571557015,1.3201347372
Cl,0,-1.948173074,0.8674042414,0.4762490439
Cl,0,-0.6610312179,1.436036845,-2.3692783738
Cl,0,-0.1766102078,4.1929710182,-1.6935595964
Cl,0,-3.028791305,3.0626401569,-1.012271969

diOHCPr-3,3,3-Trifluoropropanoate

E (total electronic) = -833.3098954
E (total electronic) + ZPVE = -833.170455
Internal Thermal Energy = -833.157490
Enthalpy = -833.156546
Gibbs Free Energy = -833.211722

C,0,1.8959487484,-0.2926842354,0.3376473936
C,0,3.1019245143,-0.8034535299,-0.3570935733
C,0,-1.6552481146,-0.8513377854,-0.2673543326
C,0,-0.4184486225,-0.1092672184,0.1730730673
O,0,-0.3890600312,0.9967538153,0.6346906734
O,0,0.6626061842,-0.8735586103,-0.021428005
C,0,2.5952501442,0.6002562737,-0.6262322936
O,0,3.2379081619,1.6972680617,-0.0681150227
O,0,4.2186549704,-1.0054538536,0.4438903354
C,0,-2.9187727052,-0.0604454681,-0.0636667827
F,0,-3.128786003,0.247570802,1.2211899193
F,0,-2.9247468875,1.0846131966,-0.7553199816
F,0,-3.9811410632,-0.7694121588,-0.4736200924
H,0,1.9985693496,-0.0425851726,1.3848029553
H,0,2.9405931168,-1.5211324321,-1.1529342012
H,0,-1.5678681937,-1.1033041306,-1.3233472038
H,0,-1.734690493,-1.7838532627,0.2895191351
H,0,2.1210921179,0.7534205062,-1.5889262702
H,0,4.0414582199,1.8767583349,-0.56681165
H,0,5.0100205862,-0.8221351326,-0.0724900702

TS–diOHCPr-Trifluoropropanoate

E (total electronic) = -833.2580715
E (total electronic) + ZPVE = -833.120963
Internal Thermal Energy = -833.107884
Enthalpy = -833.106939
Gibbs Free Energy = -833.164020

C,0,-1.2363076786,-0.1428562082,-0.0888545219
C,0,-2.3299612382,-0.9162732601,0.3018113414
C,0,-1.8020592069,1.0124803718,0.4534320474
O,0,-1.8240084124,2.1404871431,-0.2602399883
O,0,-2.8872530777,-1.7635141496,-0.5688737772
H,0,-1.0047104982,-0.1153494994,-1.1444801554
H,0,-2.6751018956,-0.9473752753,1.3248646075
H,0,-2.1198093067,1.0640227312,1.4847242953
H,0,-2.3317067751,2.822557799,0.1936517207
H,0,-3.6936746454,-2.1465351322,-0.2057326252
C,0,2.7358219573,-0.6157375988,0.4732763283
C,0,1.3928392841,-0.1052569041,-0.0490376358
O,0,1.3317543723,0.7882115108,-0.8827596869
O,0,0.3973680377,-0.715056486,0.4864577514
C,0,3.9342522639,0.0679480433,-0.1182501073
H,0,2.7719636424,-0.4858272145,1.5538164756
H,0,2.8185559363,-1.6818512866,0.2674964154
F,0,4.0217198441,-0.0837398694,-1.4465629769
F,0,5.0709176582,-0.4417084201,0.396484905
F,0,3.9639293085,1.3835834452,0.1336507366

diOHCPr-Hexafluoroisobutanoate

E (total electronic) = -1170.3836555
E (total electronic)+ZPVE = -1170.239240
Internal Thermal Energy = -1170.222773
Enthalpy = -1170.221829
Gibbs Free Energy = -1170.286382

C,0,2.3524106817,-0.4925023664,-0.4104829619
C,0,3.4540189828,0.4500173009,-0.719329451
C,0,-1.2734227828,0.0074278699,-0.5322495306
C,0,0.0572121129,-0.5799758165,-0.0680941994
O,0,0.1712594578,-1.3442476178,0.8441976116
O,0,1.0531120012,-0.0996455653,-0.8060984388
C,0,3.0142887994,0.2228291926,0.7141531931
O,0,3.7705292698,-0.5717323991,1.5635125511
O,0,4.6225007424,-0.1283845999,-1.1950572359
C,0,-1.4631096682,1.3817162554,0.1109718994
F,0,-1.2678874497,1.3404461628,1.4307065492
F,0,-0.5910551214,2.2523290178,-0.3960597599
F,0,-2.6877059127,1.85978911,-0.1023179084
C,0,-2.4270764784,-0.9398648183,-0.2203437893
F,0,-2.7199729546,-0.9817396478,1.0788058518
F,0,-2.1316177953,-2.1774752484,-0.6183228894
F,0,-3.5323617781,-0.5686203002,-0.8699157086
H,0,2.5567234373,-1.5499619567,-0.5044026583
H,0,3.1737636922,1.4046000861,-1.149209168
H,0,-1.2520818892,0.1561393316,-1.6107076975
H,0,2.4623103268,1.0370831855,1.1707920764
H,0,4.5392161502,-0.072745064,1.8584209911
H,0,5.3748921758,0.3813468877,-0.8776173268

TS–diOHCPr-Hexafluoroisobutanoate

E (total electronic) = -1170.3369788
E (total electronic)+ZPVE = -1170.194649
Internal Thermal Energy = -1170.178247
Enthalpy = -1170.177302
Gibbs Free Energy = -1170.241565

C,0,-1.1143959318,-1.8189283216,-0.2289885
C,0,-1.3894751403,-2.6568320828,-1.3120443293
C,0,0.1454864753,-2.411289454,-0.0990972041
O,0,0.55686439,-2.840010202,1.0984287373
O,0,-2.5463229758,-3.3294030804,-1.3521465715
C,0,-0.8505424312,2.1848302318,0.1196819415
C,0,-0.8738509583,0.6721732727,0.4633392329
O,0,-0.4966207922,0.2943247221,1.5578575144
O,0,-1.2855438542,-0.0433446377,-0.5120657402
C,0,-1.0024706053,3.0537958772,1.3576830106
F,0,-2.0142505919,2.6244802211,2.1154518118

F,0,-1.2838250417,4.3215501112,1.0252450079
F,0,0.095641797,3.0834855579,2.1152978815
C,0,0.4274055965,2.501504425,-0.6445648825
F,0,1.5128583383,2.0157907896,-0.032997573
F,0,0.6154673356,3.8173242357,-0.7930673946
F,0,0.3887633249,1.9665837316,-1.8664067924
H,0,-1.7701409684,-1.8976265838,0.6273142497
H,0,-0.7643948022,-2.6770826197,-2.1924744403
H,0,0.8604793739,-2.4150402037,-0.9085467175
H,0,1.3910523323,-3.3164551844,1.0216150845
H,0,-2.5556295028,-3.9470590699,-2.0918282013
H,0,-1.6834703677,2.4174942638,-0.5413701255

diOHCPr-Nonafluorotrimethylacetate

E (total electronic) = -1507.445737
E (total electronic)+ZPVE = -1507.296828
Internal Thermal Energy = -1507.277110
Enthalpy = -1507.276166
Gibbs Free Energy = -1507.346225

C,0,-1.427503455,0.3532519818,-0.7344136737
C,0,-2.5981582445,-0.3562402399,-0.1672934131
C,0,2.1693028573,0.0414576825,0.0114497414
C,0,0.8423156942,0.7209748073,-0.4206216406
O,0,0.7665166824,1.8572100967,-0.7728305377
O,0,-0.152407297,-0.1500145882,-0.3773768693
C,0,-2.2447464912,1.0426840347,0.3009286414
O,0,-2.9688195731,2.1379975539,-0.1449024473
O,0,-3.6549364222,-0.5582403939,-1.0428693221
C,0,2.351450386,-1.2458963125,-0.8437034063
C,0,3.3505280299,1.0104294339,-0.2650207166
C,0,2.1540144902,-0.33359852,1.5183304613
F,0,1.9390259245,-1.0273005761,-2.0902912977
F,0,3.6244322309,-1.621907421,-0.8980276101
F,0,3.5175856753,1.1501679556,-1.5780325494
F,0,3.1546130064,2.2087021945,0.26160022
F,0,4.4844767927,0.5359972851,0.2486192051
F,0,3.1292782442,-1.1972901257,1.792179936
F,0,2.3387628246,0.7515722181,2.2645843781
F,0,1.0075965156,-0.8864421302,1.8856657409
F,0,1.65018148,-2.2563025832,-0.3447460154
H,0,-1.5019459233,0.7217349137,-1.747906901
H,0,-2.3916742088,-1.1511951555,0.5398639035
H,0,-1.820555854,1.1096196958,1.2966260341
H,0,-3.8033092706,2.1780770406,0.3336883389
H,0,-4.4813610948,-0.5089748479,-0.5516222006

TS–diOHCPr-Nonafluorotrimethylacetate

E (total electronic) = -1507.4036363
E (total electronic)+ZPVE = -1507.257093
Internal Thermal Energy = -1507.237357
Enthalpy = -1507.236413
Gibbs Free Energy = -1507.307253

C,0,-1.3712805281,-1.5526704699,0.8861552037
C,0,-1.7129512278,-2.3721534032,-0.1937877357
C,0,-0.1134217706,-2.1676798742,0.8851330267
O,0,0.3756272496,-2.6754143028,2.0234801829
O,0,-2.8519202618,-3.0782389526,-0.153945802
C,0,-0.6380859655,2.3892925722,0.9584693715
C,0,-0.816158056,0.8941679652,1.4479834353
O,0,-0.2149948724,0.5191952279,2.4306780819
O,0,-1.5502313838,0.2134213758,0.6620329176
C,0,0.3033317155,3.1507570778,1.9218306207
C,0,-1.9818100665,3.1470195727,0.8614261151
C,0,0.0169931627,2.3158699509,-0.4429185766
F,0,-0.0734998533,3.0447305873,3.188568062
F,0,1.5472799286,2.6863119952,1.8138517554
F,0,0.3383673443,4.4583346661,1.6408752059
F,0,-1.8484075895,4.2634217464,0.1380001919
F,0,-2.4013585692,3.50050307,2.0773475374
F,0,0.9147694448,1.3306864932,-0.4861198774
F,0,0.6516212904,3.4445423396,-0.7610042789
F,0,-0.8868588805,2.0865266203,-1.3902076043
F,0,-2.9438358079,2.4301601171,0.3006850461
H,0,-1.9577482922,-1.6672314269,1.7874959168
H,0,-1.1743588251,-2.337036403,-1.1288727724
H,0,0.5463869608,-2.1152475293,0.0315398916
H,0,1.1937898002,-3.156285851,1.8561555216
H,0,-2.9050169466,-3.6783991646,-0.9059994367

diOHCPr-Cyanoacetate

E (total electronic) = -588.4678182
E (total electronic) + ZPVE = -588.334984
Internal Thermal Energy = -588.323584
Enthalpy = -588.322640
Gibbs Free Energy = -588.373916

C,0,-1.1191337375,-0.2547964965,-0.3539085284
C,0,-2.3332757012,-0.7650573281,0.3265075303
C,0,2.4219358524,-0.8852717443,0.2544884337
C,0,1.1936895012,-0.1042745588,-0.1681339049
O,0,1.1914472877,1.0168236943,-0.5883517021
O,0,0.1065611481,-0.8617208598,-0.0069318526
C,0,-1.806919671,0.6244132143,0.6303197885
O,0,-2.4308049077,1.7442306537,0.0974966931
O,0,-3.4502812691,-0.9328297945,-0.4814184331
C,0,3.6379688325,-0.0978540414,0.1125094686
N,0,4.5986941131,0.5150824708,0.0039679599
H,0,-1.2143305257,0.0211926747,-1.395170955
H,0,-2.1831242133,-1.5032868293,1.105578959
H,0,2.3055774774,-1.2004026721,1.2913939145
H,0,2.4954161048,-1.7884082227,-0.3513285981
H,0,-1.3326253243,0.7465851936,1.5973578092
H,0,-3.2314685388,1.9257079429,0.6001676761
H,0,-4.2404304287,-0.7508182968,0.0372947411

TS–diOHCPr-Cyanoacetate

E (total electronic) = -588.4179718
E (total electronic) + ZPVE = -588.287545
Internal Thermal Energy = -588.276023
Enthalpy = -588.275079
Gibbs Free Energy = -588.327633

C,0,-1.6785304293,-0.6003809627,-0.3407145193
C,0,-2.8300956863,-1.2947633462,0.0341842647
C,0,-2.1933465583,0.5896516561,0.178603053
O,0,-2.1451987923,1.7082370804,-0.5503108705
O,0,-3.428884528,-2.1055062244,-0.8448322122
H,0,-1.4304845475,-0.5965141327,-1.3931571162
H,0,-3.19032841,-1.3032540189,1.052406416
H,0,-2.5174939002,0.6720589226,1.2058227196
H,0,-2.6259654285,2.4210671794,-0.1147863569
H,0,-4.2661765834,-2.430029773,-0.4951104515
C,0,2.238926469,-1.2956125382,0.3232933276
C,0,0.934965611,-0.711321363,-0.2484543583
O,0,0.9567435936,0.1716220944,-1.0915008968
O,0,-0.1022427352,-1.2575337412,0.2705570093
C,0,3.4287413378,-0.7199395585,-0.2850872398
N,0,4.3663571189,-0.2684360232,-0.7653269488
H,0,2.2607785973,-1.1181480649,1.397969113
H,0,2.2413998713,-2.3742561858,0.1729310672

diOHCPr-Dicyanoacetate

E (total electronic) = -680.6945176
E (total electronic) + ZPVE = -680.563043
Internal Thermal Energy = -680.549960
Enthalpy = -680.549015
Gibbs Free Energy = -680.604355

C,0,-0.6551201366,-1.2434778548,0.48980617
C,0,-0.2870038481,-2.3084120469,-0.4726254991
C,0,-0.3202448687,2.4104051959,0.2883770838
C,0,-0.3406671383,1.0106077456,0.9394519738
O,0,-0.1997689673,0.835816755,2.1097186802
O,0,-0.5819333272,0.091019882,0.0197398326
C,0,0.6034680725,-2.0042811501,0.7167460358
O,0,0.6017269378,-2.8348642853,1.8273861914
O,0,-1.1068883959,-3.4275143266,-0.4690327592
C,0,0.3450397005,2.412462117,-1.0168348057
C,0,0.2865767518,3.3879559364,1.1932784258
N,0,0.8632619445,2.4140759655,-2.0360049945
N,0,0.7538128056,4.1540405028,1.9013081275
H,0,-1.4748530342,-1.4388950994,1.1668811852
H,0,0.0940378272,-1.9861459413,-1.4346925009
H,0,-1.3666705292,2.6917560615,0.1307510618
H,0,1.53379518,-1.4969477964,0.4881118869
H,0,1.1114752349,-3.6267536217,1.6275564683
H,0,-0.5746722094,-4.2046180393,-0.6683945637

TS–diOHCPr-Dicyanoacetate

E (total electronic) = -680.6520086
E (total electronic) + ZPVE = -680.522832
Internal Thermal Energy = -680.509662
Enthalpy = -680.508718
Gibbs Free Energy = -680.565084

C,0,-0.7604408786,-1.7026348475,-0.3958794027
C,0,-0.6336453206,-2.4064290504,-1.5973860346
C,0,0.3851805728,-2.3657155514,0.0586062689
O,0,0.3659730634,-2.9768701335,1.250069937
O,0,-1.6954257474,-3.0559933783,-2.0951876059
H,0,-1.665246257,-1.8746795732,0.1715545792
H,0,0.2426498049,-2.3187639531,-2.2221963517
H,0,1.3359087546,-2.2728876541,-0.444928036
H,0,1.1788917473,-3.4755428908,1.3884099247
H,0,-1.441396434,-3.5893751675,-2.856371619
C,0,-0.9046679656,2.212822961,0.5448052507
C,0,-0.8598804796,0.643190987,0.6612856316
O,0,-0.889741989,0.1405514506,1.7629749531
O,0,-0.8371081182,0.0826493528,-0.4816129067
C,0,-0.5465959558,2.8518390588,1.809459242
N,0,-0.2702915567,3.3443597276,2.8045314223
C,0,-0.0691251756,2.7068585712,-0.5480308045
N,0,0.5885014285,3.0867602063,-1.4040381524
H,0,-1.9442544934,2.4629638845,0.3156277039

diOHCPr-Tricyanoacetate

E (total electronic) = -772.9069935
E (total electronic) + ZPVE = -772.777806
Internal Thermal Energy = -772.762649
Enthalpy = -772.761705
Gibbs Free Energy = -772.822726

C,0,-1.1385342442,-0.2651082733,-0.369181369
C,0,-2.3371059974,-0.7603277492,0.3457819666
C,0,2.4334871008,-0.9417421742,0.2810063649
C,0,1.1664858777,-0.111412907,-0.1704990674
O,0,1.2462525442,1.0031793695,-0.5661720666
O,0,0.102737932,-0.8688311437,-0.0257198571
C,0,-1.8043487573,0.6354430979,0.6106450288
O,0,-2.4276673838,1.7438861914,0.0600693254
O,0,-3.4631430391,-0.9483662852,-0.4401348752
C,0,3.6310160357,-0.0976153849,0.1568658727
N,0,4.5589897186,0.5608883813,0.059175909
H,0,-1.2367237302,-0.0181409355,-1.4167893953
H,0,-2.1682858669,-1.4786362048,1.1396344087
H,0,-1.314244086,0.7742477865,1.5678045532
H,0,-3.227428352,1.9356720542,0.560892258
H,0,-4.2465869272,-0.7628607885,0.0878284194
C,0,2.5561007804,-2.1274483496,-0.5857416642
C,0,2.2510438523,-1.3656264627,1.680575952
N,0,2.6379192727,-3.0376880184,-1.2714877763
N,0,2.0926781195,-1.6787076236,2.7679496725

TS–diOHCPr-Tricyanoacetate

E (total electronic) = -772.8711296
E (total electronic) + ZPVE = -772.744404
Internal Thermal Energy = -772.729146
Enthalpy = -772.728201
Gibbs Free Energy = -772.789834

C,0,1.9862344686,0.1028751072,-0.2343613231
C,0,2.9970966459,0.909401567,0.3037603534
C,0,2.5870093805,-0.9300324907,0.5003114559
O,0,2.9258649569,-2.0686865691,-0.1258710086

O,0,3.7538398744,1.6490835842,-0.5239540985
H,0,1.9890811571,-0.0163819831,-1.3098623589
H,0,3.0679287561,1.1049686191,1.3629888502
H,0,2.6149412233,-0.9199129688,1.5796230596
H,0,3.422080346,-2.6444481898,0.4663527904
H,0,4.4769397867,2.0637609216,-0.0407466273
C,0,-2.0386655551,0.1329086628,0.0591975147
C,0,-0.5262892588,-0.3014963138,-0.3782413119
O,0,-0.3874939111,-1.3493137866,-0.9467771774
O,0,0.3017107474,0.5750182382,0.0057472516
C,0,-3.0115848493,-0.7510772586,-0.5897129527
N,0,-3.7560233722,-1.4474016048,-1.1069547962
C,0,-2.271395687,1.5290981208,-0.3287573778
C,0,-2.1115899722,-0.0081244919,1.5192285766
N,0,-2.4360645606,2.6144129213,-0.6484361953
N,0,-2.1321465767,-0.1348121851,2.6555760754

diOHCPr-Nitroacetate

E (total electronic) = -700.7296405
E (total electronic) + ZPVE = -700.592205
Internal Thermal Energy = -700.580063
Enthalpy = -700.579119
Gibbs Free Energy = -700.632825

C,0,-1.5124496907,-0.316816018,-0.3219910069
C,0,-2.7314557309,-0.7131846018,0.4226219545
C,0,2.0148648271,-0.8759326109,0.4082683462
C,0,0.7984512775,-0.1593459241,-0.1425667833
O,0,0.8247138149,0.8890369431,-0.7187012395
O,0,-0.2906173894,-0.8785998891,0.1133241385
C,0,-2.1915394868,0.7001693064,0.5259139539
O,0,-2.8036201191,1.7381811163,-0.1622615571
O,0,-3.84895227,-0.9829972234,-0.3556286494
N,0,3.2123338354,-0.04806926,0.0934743412
O,0,3.7608549408,-0.2471173842,-0.9647653846
O,0,3.5370268698,0.7871255198,0.9042720904
H,0,-1.6014751237,-0.19365172,-1.3924939907
H,0,-2.5884108872,-1.3339427494,1.2994037151
H,0,1.9448528634,-0.9719285221,1.4870977284
H,0,2.1379360985,-1.8425217108,-0.0694094067
H,0,-1.7162649905,0.9537343668,1.4666076472
H,0,-3.6055834005,1.9937702388,0.3049308643
H,0,-4.6369344386,-0.7066158773,0.1232602387

TS–diOHCPr-Nitroacetate

E (total electronic) = -700.6826588
E (total electronic) + ZPVE = -700.547446
Internal Thermal Energy = -700.535305
Enthalpy = -700.534360
Gibbs Free Energy = -700.588695

C,0,-0.7760718477,-1.6570311277,-0.4175119007
C,0,-1.3025253615,-2.4667808335,-1.4264709744
C,0,0.4346344717,-2.3520026051,-0.4900324481
O,0,1.0088090816,-2.8021710369,0.6303008875
O,0,-2.5051780308,-3.0307339255,-1.2624136485
H,0,-1.2820566999,-1.6783718194,0.5380955955
H,0,-0.8369697882,-2.5477686675,-2.3974346516
H,0,0.9988926393,-2.4233261347,-1.4083045498
H,0,1.775235561,-3.3488116267,0.4242261117
H,0,-2.6948977971,-3.6449567422,-1.9804123904
C,0,-0.4675707047,2.3254146173,-0.0140673619
C,0,-0.4211099901,0.8209483998,0.2999696905
O,0,-0.0229670882,0.4206624104,1.38001526
O,0,-0.8368838785,0.126213787,-0.6907548049
N,0,0.0304619409,3.0805881858,1.1635327019
O,0,-0.7771963378,3.4047874149,2.0054011922
O,0,1.2204418026,3.2938393139,1.2311460405
H,0,0.1817696063,2.554606432,-0.8518725517
H,0,-1.4884595789,2.6401639582,-0.2005891979

diOHCPr-Dinitroacetate

E (total electronic) = -905.2167016
E (total electronic) + ZPVE = -905.076671
Internal Thermal Energy = -905.062108
Enthalpy = -905.061163
Gibbs Free Energy = -905.120546

C,0,1.1524305503,-0.557690031,-0.616385734
C,0,2.2085747068,0.4816270396,-0.6135035585
C,0,-2.4686296155,-0.1107988216,-0.7082402368
C,0,-1.1410270125,-0.7945467565,-0.371134438
O,0,-1.0626436937,-1.7677429096,0.3124883535
O,0,-0.1583091896,-0.1258375624,-0.9441109959
C,0,1.7388284389,-0.1423509452,0.6867639198
O,0,2.5092271549,-1.1027667887,1.3241420356
O,0,3.4185792981,0.1047147821,-1.1765718627
N,0,-3.5891224964,-1.0072973429,-0.2575834989
O,0,-3.7998598404,-1.9446811542,-0.9794662433
O,0,-4.1433030632,-0.7417080949,0.7761746696
N,0,-2.5903529688,1.1865412608,0.0523306106
O,0,-1.8572702398,1.3356523782,0.9969180099
O,0,-3.4273212622,1.9521603181,-0.3451619202
H,0,1.4085991654,-1.5408056671,-0.9853320114
H,0,1.8876420428,1.5027025313,-0.7836202742
H,0,-2.6008347117,0.0948082935,-1.7650020207
H,0,1.1283598861,0.4937028714,1.3183341502
H,0,3.2378143918,-0.6680774777,1.7793481866
H,0,4.1328284589,0.5475980767,-0.7068721413

TS– diOHCPr-Dinitroacetate

E (total electronic) = -905.1756538
E (total electronic) + ZPVE = -905.037977
Internal Thermal Energy = -905.023288
Enthalpy = -905.022344
Gibbs Free Energy = -905.083135

C,0,-0.7432357763,-1.4948959954,-0.4199782426
C,0,-0.6445385283,-2.0741499364,-1.6893905485
C,0,0.501340558,-2.0714715147,-0.1356622195
O,0,0.6490629237,-2.808840105,0.972992729
O,0,-1.6647343894,-2.8058812506,-2.1615016275
H,0,-1.5706239491,-1.8191753095,0.1965698356
H,0,0.1517522594,-1.8180505088,-2.3721591034

H,0,1.3898864133,-1.8136348545,-0.6928889973
H,0,1.5188776699,-3.2231751685,0.9906069801
H,0,-1.4220368559,-3.2306488944,-2.9916410101
C,0,-0.4510248859,2.3259903147,0.5999467384
C,0,-0.5747766819,0.784862508,0.7479702827
O,0,-0.2520592358,0.2584702898,1.7900388868
O,0,-1.0041938863,0.2661907583,-0.3320373578
N,0,-0.1431319389,2.9332954018,1.9343779733
O,0,-1.0906076304,3.0458637815,2.6683797593
O,0,1.0012212543,3.2150438227,2.1856743382
N,0,0.6927831218,2.6676137958,-0.3193143521
O,0,0.6565799473,3.7597216715,-0.8285187671
O,0,1.5564835334,1.8397211336,-0.459607748
H,0,-1.3471539228,2.79850306,0.2155554507

diOHCPr-Trinitroacetate

E (total electronic) = -1109.6851688
E (total electronic)+ZPVE = -1109.543840
Internal Thermal Energy = -1109.526607
Enthalpy = -1109.525662
Gibbs Free Energy = -1109.592223

C,0,-0.6392219316,-1.2499848551,0.5754851527
C,0,-1.1912892618,-2.0568936034,-0.5361645974
C,0,0.5688716259,2.2358610523,0.5675113525
C,0,0.4448694177,0.7467626606,0.9941999842
O,0,1.2099750055,0.2929523509,1.7828692718
O,0,-0.5208867726,0.149852655,0.3441637474
C,0,0.2709668372,-2.1785762449,-0.1481824052
O,0,0.7158133629,-3.2617702618,0.5924099839
O,0,-2.1021080717,-3.0337007524,-0.1664019448
N,0,1.3459576309,2.9663097648,1.6521419653
O,0,0.8394231301,2.9291512679,2.735173443
O,0,2.3799495207,3.481687708,1.3268961907
N,0,-0.7437109661,2.9718923478,0.2955928368
N,0,1.3754631052,2.331557327,-0.726859529
O,0,-1.0204184096,3.8940194877,1.0063304812
O,0,-1.3555798237,2.5447746399,-0.6419863535
O,0,2.0497824768,1.3724273885,-0.9823771113
O,0,1.2757706488,3.3577169056,-1.3349163559
H,0,-0.9178662173,-1.5110730976,1.586469961
H,0,-1.3813195365,-1.5368092774,-1.4677866069
H,0,0.9766356916,-1.7365208489,-0.8428634549
H,0,0.7757954964,-4.0323864243,0.0180311436
H,0,-2.0260799589,-3.7768271904,-0.7738391553

TS–diOHCPr-Trinitroacetate

E (total electronic) = -1109.6501663
E (total electronic)+ZPVE = -1109.511161
Internal Thermal Energy = -1109.493826
Enthalpy = -1109.492882
Gibbs Free Energy = -1109.560959

C,0,2.5953486545,0.1348228027,-0.3413599694
C,0,3.5441354048,0.8957994178,0.3543608869
C,0,3.0945769474,-0.9334883625,0.4193421216
O,0,3.5091677027,-2.0456237345,-0.2090957587
O,0,4.415106438,1.6507675949,-0.3370226273
C,0,-1.3905152649,0.0547399277,-0.0431042304
C,0,0.099996573,-0.3358245702,-0.4291859571
O,0,0.2690960741,-1.4834388631,-0.7555164665
O,0,0.9029384542,0.6296834147,-0.291297352
N,0,-2.3127419775,-0.8698855396,-0.8090639508
O,0,-2.2635615432,-0.7651657839,-2.0011836232
O,0,-2.9517850388,-1.6588097857,-0.1643543668
N,0,-1.7220590125,1.5166600604,-0.2884823537
N,0,-1.6346812723,-0.1785279406,1.4421902639
O,0,-2.6571641271,0.2680394741,1.884010252
O,0,-0.7894105478,-0.8009760685,2.024182976
O,0,-1.2395374928,2.2605929953,0.5218692033
O,0,-2.3875858041,1.8042182306,-1.2422484499
H,0,2.7282035888,0.059508008,-1.4123635918
H,0,3.4757252973,1.0527047858,1.4200670845
H,0,2.9785711642,-0.9726094252,1.4922925514
H,0,3.9162105097,-2.6543475179,0.4170529085
H,0,5.074276272,2.0303798798,0.2543494494

diOHCPr-2-Cyanopropenoate

E (total electronic) = -626.5477507
E (total electronic) + ZPVE = -626.409607
Internal Thermal Energy = -626.397534
Enthalpy = -626.396590
Gibbs Free Energy = -626.448988

C,0,0.3119486688,-1.4300758829,0.3683933879
C,0,0.9136732536,-2.3027665192,-0.6676619097
C,0,-0.4801983484,0.7188093705,0.7698709594
O,0,-0.0165004753,0.7201565288,1.8759251198
O,0,-0.3980103234,-0.30042686,-0.0882202882
C,0,1.7945017073,-1.4632780531,0.2375960506
O,0,2.4742756795,-2.0501070951,1.2959464653
O,0,0.7857743683,-3.6685875668,-0.4526871063
C,0,-1.2339976702,1.8690454863,0.1819800004
C,0,-1.4318001087,2.9718532765,0.8976492629
C,0,-1.7307834029,1.7500281155,-1.1591077101
N,0,-2.1308274689,1.6639417805,-2.2306701305
H,0,-0.1059912717,-1.9109810236,1.2421200389
H,0,0.8401337707,-1.9641616054,-1.6945406936
H,0,2.2667968299,-0.6061124593,-0.2284235996
H,0,3.2399595845,-2.5222424314,0.9531450743
H,0,1.5633653813,-4.1135029822,-0.8047845457
H,0,-1.0427331984,3.0249918876,1.9049447289
H,0,-1.9721379758,3.8169230334,0.4978938954

TS–diOHCPr-2-Cyanopropenoate

E (total electronic) = -626.4981765
E (total electronic) + ZPVE = -626.362421
Internal Thermal Energy = -626.350194
Enthalpy = -626.349249
Gibbs Free Energy = -626.403363

C,0,-1.8250279556,-0.2320793479,-0.6055071877
C,0,-2.9402418469,-0.9837852564,-0.2311050217
C,0,-2.3556570621,0.9011752504,0.0156313523

O,0,-2.3816177435,2.0667873463,-0.6371342107
O,0,-3.5582408806,-1.7479545549,-1.1384630229
H,0,-1.6230571986,-0.1489103678,-1.6644814574
H,0,-3.2516747752,-1.0745963906,0.7990765065
H,0,-2.6306959756,0.9025279922,1.060142617
H,0,-2.8665390963,2.7298429516,-0.1330056064
H,0,-4.3692577831,-2.1214406042,-0.7756276727
C,0,0.790530039,-0.2189413831,-0.5624692425
O,0,0.7500790552,0.7481080423,-1.3084936357
O,0,-0.2074325849,-0.8810096709,-0.1038637777
C,0,3.276846902,-0.1834058029,-0.4925715446
C,0,2.1388057267,-0.7397580655,-0.0925177107
C,0,2.1467323488,-1.863474069,0.8009892789
N,0,2.157992753,-2.7612824138,1.516479327
H,0,4.2394588544,-0.5495876531,-0.166464714
H,0,3.2355152234,0.6616429975,-1.165761277

diOHCPr-2-Hydroxyethanoate

E (total electronic) = -571.4473834
E (total electronic) + ZPVE = -571.308713
Internal Thermal Energy = -571.297694
Enthalpy = -571.296750
Gibbs Free Energy = -571.346278

C,0,-0.8257504864,-0.2536572105,-0.3464794394
C,0,-2.0268566707,-0.8189352107,0.3130572824
C,0,2.7588319858,-0.7046730124,0.2732535934
C,0,1.481028798,-0.0247263211,-0.1474484703
O,0,1.4412358404,1.0985163911,-0.578063794
O,0,0.4184211762,-0.8137682206,0.0104184149
C,0,-1.5616688782,0.5877140071,0.6365755133
O,0,-2.2257024711,1.6858589065,0.1062746889
O,0,-3.1269665551,-1.0232784364,-0.5100939875
O,0,3.8588337126,0.1437129272,0.0854511888
H,0,-0.920601498,0.028792749,-1.3861175848
H,0,-1.8570985082,-1.5582269589,1.0870796431
H,0,2.8661633661,-1.6198506873,-0.3132430707
H,0,2.659854598,-0.9916638222,1.3227531462
H,0,-1.105456728,0.720405229,1.6109096337
H,0,-3.0457270914,1.8203915663,0.5920879915
H,0,-3.9298748628,-0.8784521389,0.0006039712
H,0,3.5220632729,0.9772162428,-0.2688737208

TS–diOHCPr-2-Hydroxyethanoate

E (total electronic) = -571.3960016
E (total electronic) + ZPVE = -571.259141
Internal Thermal Energy = -571.248336
Enthalpy = -571.247391
Gibbs Free Energy = -571.297304

C,0,2.1591366861,-4.9077944576,0.3357660694
C,0,1.1143865611,-5.6401658623,-0.229337815
C,0,3.0960406811,-5.5146555314,-0.5028957175
O,0,4.2331990991,-5.9938865826,0.0067753454
O,0,0.2234812828,-6.2438353395,0.5634154201
C,0,2.708425097,-0.9445705804,0.9858698271
C,0,2.8530820074,-2.4618918959,0.9997875002
O,0,3.7834156576,-2.9596566456,1.6328930682
O,0,1.9653755757,-3.0953749098,0.3282233855
O,0,3.7257588487,-0.3371108293,1.744965316
H,0,2.3202654423,-5.0215122488,1.3987750381
H,0,0.9232695638,-5.6409444041,-1.2924780848
H,0,2.9917312105,-5.5045673222,-1.5782415462
H,0,4.7333082628,-6.4733184952,-0.6633295488
H,0,-0.3717538504,-6.799813311,0.0482064254
H,0,2.7459961003,-0.6074243232,-0.0522942964
H,0,1.7239513739,-0.6907538834,1.3848810852
H,0,4.2596514,-1.0728963775,2.0808225284

diOHCPr-2-Hydroxypropanoate

E (total electronic) = -610.7596168
E (total electronic) + ZPVE = -610.592937
Internal Thermal Energy = -610.580503
Enthalpy = -610.579559
Gibbs Free Energy = -610.633024

C,0,-0.8749193961,0.2629780163,-0.7403684991
C,0,-1.9772895447,-0.6008087275,-0.2536475025
C,0,2.7756914916,-0.0972072939,-0.5327885117
C,0,1.4267753847,0.5852113863,-0.6230910658
O,0,1.287167775,1.7813198753,-0.6103303041
O,0,0.4226263861,-0.2879269236,-0.7070905769
C,0,-1.5483472697,0.6190953982,0.5382895164
O,0,-2.3145824804,1.7766951383,0.5123243971
O,0,-3.1437562584,-0.5720122952,-1.0072598538
C,0,2.876989923,-0.9101015364,0.7519003949
O,0,3.7915995238,0.8756103391,-0.5963518992
H,0,-1.0833110292,0.8998677077,-1.5891885157
H,0,-1.6977537511,-1.5582603504,0.1702797713
H,0,2.8603521185,-0.7631847081,-1.395201865
H,0,-1.0020907943,0.41869531,1.4531144374
H,0,-3.0839076437,1.6554626934,1.07813132
H,0,-3.8980678901,-0.6785301383,-0.4188196601
H,0,3.8688547742,-1.3530302889,0.8094868972
H,0,2.7303771104,-0.2635886679,1.6169514359
H,0,2.1335862425,-1.7042580306,0.7666481339
H,0,3.366321328,1.7431070961,-0.5796930504

TS–diOHCPr-2-Hydroxypropanoate

E (total electronic) = -610.7079058
E (total electronic) + ZPVE = -610.543093
Internal Thermal Energy = -610.530890
Enthalpy = -610.529945
Gibbs Free Energy = -610.583440

C,0,-0.9578971631,-1.97753141,-0.1036416231
C,0,-1.382155477,-2.7532629056,-1.1831925292
C,0,0.2718648518,-2.6368079456,-0.0542495393
O,0,0.7488873336,-3.06990159,1.115078747
O,0,-2.6008953215,-3.3015134737,-1.1672966827
H,0,-1.5592215933,-2.0119221635,0.7941900218
H,0,-0.8069465662,-2.832253839,-2.0941376497
H,0,0.9180706496,-2.7059877703,-0.9171456095
H,0,1.5503251216,-3.5897087295,0.9864835184

H,0,-2.719620913,-3.8943392578,-1.9178407005
C,0,-0.8069124536,2.0366339761,0.5155898474
C,0,-0.7983669652,0.5176343194,0.7130116724
O,0,-0.5863299286,0.0692532146,1.8403463245
O,0,-1.0126456582,-0.1710020483,-0.3451971101
C,0,0.2917993602,2.465274834,-0.4447910266
O,0,-0.649523818,2.6719686661,1.7675293493
H,0,-1.7817922959,2.3016539716,0.0968877964
H,0,0.2884470801,3.5496227882,-0.5417295528
H,0,1.2646819876,2.1530055778,-0.063519314
H,0,0.1364487852,2.0224858617,-1.4263517907
H,0,-0.5416630159,1.9502169236,2.4054858509

diOHCPr-2,3-Dihydroxypropanoate

E (total electronic) = -685.9867131
E (total electronic) + ZPVE = -685.814638
Internal Thermal Energy = -685.801175
Enthalpy = -685.800230
Gibbs Free Energy = -685.855874

C,0,-1.144844507,-0.9032703402,0.0118666659
C,0,-0.7479157483,-1.6631085512,-1.1982881273
C,0,-0.6187737452,2.6178508227,0.9148571009
C,0,-0.8218339126,1.1259544515,1.1013027592
O,0,-0.7797633604,0.5821735316,2.1729959169
O,0,-1.0331919802,0.5008259251,-0.0570710478
C,0,0.0939129086,-1.7261689842,0.0613681972
O,0,0.0419487397,-2.8426830624,0.88490367
O,0,-1.5753743673,-2.7248723773,-1.5411984954
C,0,0.6254345341,2.8519083349,0.0728090841
O,0,-0.526194429,3.2386064228,2.1701417133
O,0,1.6807453669,2.1147696947,0.6639780421
H,0,-1.9938279011,-1.2712148616,0.5716233851
H,0,-0.3263933827,-1.092846946,-2.0178759429
H,0,-1.4811517785,3.0167139824,0.3765081675
H,0,1.0368970165,-1.192223113,0.0254593894
H,0,0.5614106852,-3.549260693,0.4880126337
H,0,-1.0384397726,-3.4300811007,-1.9165946747
H,0,0.4364227647,2.5224082517,-0.9506545117
H,0,0.8375821159,3.9225263692,0.0720162197
H,0,-0.3753833416,2.5472534455,2.827641622
H,0,2.4957820947,2.2899347974,0.1865492329

TS–diOHCPr-2,3-Dihydroxypropanoate

E (total electronic) = -685.9352188
E (total electronic) + ZPVE = -685.765123
Internal Thermal Energy = -685.751825
Enthalpy = -685.750880
Gibbs Free Energy = -685.807348

C,0,-2.5922832404,-3.2685934506,0.3319643029
C,0,-2.7844850019,-3.8863049186,-0.9042134569
C,0,-1.3907917512,-3.9512349462,0.5336515981
O,0,-1.1547828799,-4.5540402419,1.7010235613
O,0,-3.9750592767,-4.4149290371,-1.2040499358
C,0,-2.3745981863,0.6168976603,1.4862580922
C,0,-2.4711269746,-0.9144740248,1.4816859953
O,0,-2.4000207795,-1.5111136768,2.5546886066
O,0,-2.6174161956,-1.4445561041,0.3263266806
C,0,-1.1811657656,1.0682789045,0.6670629102
O,0,-2.2915880801,1.0829604943,2.8123198684
O,0,-0.0305801904,0.3937986443,1.151833553
H,0,-3.3598403637,-3.4136017589,1.0793097853
H,0,-2.0396639665,-3.8491728536,-1.6855526289
H,0,-0.5845023635,-3.9117927844,-0.1845411679
H,0,-0.3400797247,-5.0676933691,1.6627983345
H,0,-3.9343789162,-4.9012120174,-2.0352089482
H,0,-3.2779840601,1.0101579483,1.012119839
H,0,-1.0737359107,2.1500241664,0.7748712714
H,0,-1.3616268023,0.8300843988,-0.3829760993
H,0,-2.2361025007,0.2843225082,3.3585058504
H,0,0.7388869307,0.7021944586,0.6669279876

diOHCPr-Oxoethanoate

E (total electronic) = -570.2219063
E (total electronic) + ZPVE = -570.106910
Internal Thermal Energy = -570.096527
Enthalpy = -570.095583
Gibbs Free Energy = -570.143841

C,0,-0.4850266721,-0.5818182927,-0.4432166804
C,0,0.0098950493,-1.299879339,-1.6410974898
C,0,-0.3154113457,1.4022757013,0.7411805724
O,0,-0.3754244363,0.8438585115,1.8011742083
O,0,-0.367885242,0.825468622,-0.4505514245
C,0,0.7417042682,-1.4162102715,-0.3175210726
O,0,0.6100550903,-2.5584946058,0.4597033749
O,0,-0.7923948326,-2.3386928202,-2.0936080869
C,0,-0.1683433433,2.9239979427,0.6544314045
O,0,-0.1026127758,3.514563671,-0.3813797951
H,0,-1.3786290357,-0.9625491228,0.0322479213
H,0,0.5052970506,-0.7032964772,-2.3981917286
H,0,1.6890727941,-0.8929615105,-0.2568066939
H,0,1.1465934293,-3.2608521609,0.0780145533
H,0,-0.2316012527,-3.0261746718,-2.4670838577
H,0,-0.1295757458,3.408753824,1.6399047946

TS–diOHCPr-Oxoethanoate

E (total electronic) = -570.1736715
E (total electronic) + ZPVE = -570.061053
Internal Thermal Energy = -570.050516
Enthalpy = -570.049572
Gibbs Free Energy = -570.099688

C,0,-1.2384766081,-0.2707109859,-0.3889364802
C,0,-2.2115831002,-1.1989786265,-0.012770002
C,0,-1.8507609429,0.7073051916,0.3994653458
O,0,-2.0916071235,1.918477521,-0.1119973868
O,0,-2.8174469215,-1.9380328423,-0.9492208427
H,0,-1.1560447846,-0.0513640193,-1.4447254389
H,0,-2.4022290032,-1.4419587206,1.0222106131
H,0,-2.0190761315,0.5653945675,1.4567966515
H,0,-2.6061463852,2.4524222447,0.5037155596
H,0,-3.5360977253,-2.4537194195,-0.5665425583

C,0,1.3325543837,0.1144918467,-0.5272077633
O,0,1.1153427201,1.1668152076,-1.1132191135
O,0,0.4853857665,-0.7401941555,-0.1039882751
C,0,2.8132290921,-0.2301409046,-0.2600261841
O,0,3.1785819817,-1.2176783897,0.3101044717
H,0,3.5145667817,0.5265314847,-0.6478155967

diOHCPr-2-Oxopropanoate

E (total electronic) = -609.544212
E (total electronic) + ZPVE = -609.401554
Internal Thermal Energy = -609.389500
Enthalpy = -609.388556
Gibbs Free Energy = -609.441075

C,0,-1.0532981775,-0.1456938885,-0.3887750793
C,0,-2.1864644228,-0.8866950882,0.2132801303
C,0,1.2216199489,0.2553427876,-0.2164640829
O,0,1.0844557152,1.4076719616,-0.5209024436
O,0,0.2419075813,-0.6357008803,-0.1202812474
C,0,-1.8308282828,0.5042608543,0.7022432473
O,0,-2.5962326947,1.5979815945,0.3212091219
O,0,-3.2866789752,-1.0792191065,-0.6120042135
C,0,2.6014610125,-0.3607284678,0.108051671
O,0,2.6780684512,-1.5133694536,0.4351949074
C,0,3.7531584489,0.5788267468,-0.0202626188
H,0,-1.1942261184,0.2549941981,-1.3833963443
H,0,-1.9375050336,-1.6982050102,0.8870548876
H,0,-1.3625780533,0.5549385933,1.6785188413
H,0,-3.4176426152,1.5963963034,0.8232383479
H,0,-4.0857635592,-1.0592314211,-0.0757519701
H,0,3.7889029331,0.9717485574,-1.0365989663
H,0,3.6015188846,1.431418476,0.642006602
H,0,4.675822957,0.0632772431,0.2239102093

TS–diOHCPr-2-Oxopropanoate

E (total electronic) = -609.4942161
E (total electronic) + ZPVE = -609.353457
Internal Thermal Energy = -609.341510
Enthalpy = -609.340566
Gibbs Free Energy = -609.394005

C,0,-1.0319351967,-0.0617220795,-0.0800786615
C,0,-1.9918667081,-1.0076061584,0.2841402579
C,0,-1.6466211652,0.9085942173,0.7147821331
O,0,-1.8829109191,2.1251427814,0.2155167706
O,0,-2.5770761953,-1.7527636572,-0.6595389821
H,0,-0.9440833669,0.166748874,-1.1334102664
H,0,-2.1924037071,-1.2543323918,1.3163864718
H,0,-1.8248658454,0.7543881583,1.768923188
H,0,-2.3989063737,2.6540534373,0.8343953945
H,0,-3.2877180528,-2.284503401,-0.284148648
C,0,1.5479620206,0.2939632851,-0.2943428488
O,0,1.3134323296,1.3132395806,-0.9306188355
O,0,0.7003633724,-0.519552441,0.2055104878
C,0,3.0396231994,-0.0862417629,-0.0432245461
O,0,3.3198629161,-1.0467998117,0.6268613734
C,0,4.056531223,0.8098160123,-0.6781382588
H,0,3.8947839584,0.8366072223,-1.7556204225
H,0,3.9183897417,1.8287295568,-0.3172267097
H,0,5.0566996691,0.4550437481,-0.4498535679

diOHCPr-3-Oxopropanoate

E (total electronic) = 609.5447828
E (total electronic) + ZPVE = -609.401566
Internal Thermal Energy = -609.389782
Enthalpy = -609.388838
Gibbs Free Energy = -609.441175

C,0,-1.0913615991,0.0069800349,-0.6587827501
C,0,-2.0585900448,-0.7944114026,0.1301943591
C,0,2.5529115816,-0.1773379625,-0.803338106
C,0,1.1862859107,0.4407328143,-0.8849293836
O,0,0.9669176171,1.6106862081,-1.0423955266
O,0,0.2273940256,-0.4823329235,-0.7214668875
C,0,-1.596746293,0.5610320039,0.6270990795
O,0,-2.4322976147,1.6654013475,0.5205539187
O,0,-3.3226527907,-0.9395595982,-0.4281439326
C,0,2.98059959,-0.330965654,0.6356063402
O,0,2.3096913042,0.0119944913,1.5727444544
H,0,-1.4566044458,0.4750914931,-1.5627327923
H,0,-1.6633794726,-1.6519163679,0.6622124241
H,0,2.5741800026,-1.1622227742,-1.271294034
H,0,3.2801000639,0.4558441556,-1.3109802936
H,0,-0.9106748501,0.5495228857,1.466604437
H,0,-3.1174055052,1.6058340075,1.194082671
H,0,-3.9746742138,-0.960673155,0.2796103422
H,0,3.9728977341,-0.783815604,0.7800466799

TS–diOHCPr-3-Oxopropanoate

E (total electronic) = -609.4903652
E (total electronic) + ZPVE = -609.349154
Internal Thermal Energy = -609.337440
Enthalpy = -609.336496
Gibbs Free Energy = -609.389190

C,0,-0.477150325,-1.5885040811,-0.292092675
C,0,-0.5962980325,-2.2084763796,-1.5358715128
C,0,0.7371338668,-2.2197189671,-0.018600163
O,0,0.94227457,-2.7826312467,1.1731903613
O,0,-1.7610906248,-2.754860617,-1.8952770315
H,0,-1.2754845656,-1.748702672,0.4187092327
H,0,0.18875661,-2.1660227435,-2.2768448548
H,0,1.572049344,-2.1731710611,-0.7027402882
H,0,1.7784317444,-3.2619270335,1.1859943775
H,0,-1.6726243107,-3.2354514655,-2.7259318843
C,0,-0.5691191137,2.2938205226,0.8625834739
C,0,-0.6104993825,0.7734530366,0.8659228286
O,0,-0.6613656498,0.1649410598,1.9307858821
O,0,-0.5588645983,0.2402293617,-0.3024374449
C,0,0.8407475486,2.8128748902,0.8714791873
O,0,1.825579405,2.1196933341,0.8965009659
H,0,-1.066244913,2.7084034567,-0.015978631
H,0,-1.0698400553,2.6937817222,1.7462794221
H,0,0.9324324824,3.9112188832,0.8567477542

diOHCPr-2-Oxobutanoate

E (total electronic) = -648.8524721
E (total electronic) + ZPVE = -648.681036
Internal Thermal Energy = -648.667728
Enthalpy = -648.666784
Gibbs Free Energy = -648.722558

C,0,-0.291233466,-1.9575421986,0.4840512748
C,0,-1.2978622887,-2.9143354515,-0.0328214404
C,0,0.441944023,0.2358879053,0.3432566777
O,0,1.5909045176,-0.1004277243,0.4219553283
O,0,-0.6011423493,-0.5862161564,0.3712454952
C,0,0.0308195212,-2.7380632894,-0.7425004055
O,0,1.0323623321,-3.6889550317,-0.6003343542
O,0,-1.5272114498,-4.0337847855,0.756425322
C,0,0.0112441676,1.7132795248,0.199526351
O,0,-1.1545285637,1.989978779,0.1199017062
C,0,1.1366263577,2.6991169787,0.1709270184
C,0,0.6601058745,4.1319470583,0.0296819224
H,0,0.2421311455,-2.2343857145,1.3832793336
H,0,-2.1587427724,-2.4924609318,-0.5382179182
H,0,-0.0060330132,-2.2085416899,-1.687604349
H,0,0.8109638238,-4.4600255364,-1.1325029632
H,0,-1.7299228263,-4.7813725099,0.1849488368
H,0,1.7216095092,2.5463466263,1.0815969994
H,0,1.8031838858,2.403435709,-0.6435089309
H,0,0.0159805876,4.4094910681,0.862333229
H,0,1.5096637434,4.8106941862,0.0097800316
H,0,0.0924192405,4.2619901844,-0.8901291651

TS–diOHCPr-2-Oxobutanoate

E (total electronic) = -648.8022236
E (total electronic) + ZPVE = -648.632711
Internal Thermal Energy = -648.619505
Enthalpy = -648.618561
Gibbs Free Energy = -648.674911

C,0,-1.8852976874,-0.0713155754,-0.1152517339
C,0,-2.9214336927,-0.9643411728,0.1632287677
C,0,-2.488634847,0.9181269005,0.6644191569
O,0,-2.616490786,2.15798317,0.1835434188
O,0,-3.4876094529,-1.6519145897,-0.8341127373
H,0,-1.7156930901,0.1741930765,-1.1546421955
H,0,-3.203486728,-1.2198423182,1.1740781274
H,0,-2.7445100308,0.7519231919,1.7006097329
H,0,-3.1372997169,2.7047529838,0.782559071
H,0,-4.2516317548,-2.1470399237,-0.5181862141
C,0,0.7214704092,0.1251610042,-0.1619546534
O,0,0.5884169498,1.1699666454,-0.7862648169
O,0,-0.204730859,-0.642646514,0.2662977389
C,0,2.1679128178,-0.3565773016,0.1693767806
O,0,2.3436814767,-1.3535148166,0.8217445812
C,0,3.2816123948,0.4932178359,-0.3704803831
C,0,4.6594324334,-0.0306462732,-0.0125666861
H,0,3.1368700654,0.5638865534,-1.451263684
H,0,3.1191593809,1.5085780807,-0.0017144565
H,0,5.4309262083,0.6161113622,-0.425484059
H,0,4.7891288715,-0.0742139502,1.0677656113
H,0,4.8068217977,-1.0356225491,-0.4051561668

diOHCPr-3-Oxobutanoate

E (total electronic) = -648.8656941
E (total electronic) + ZPVE = -648.694383
Internal Thermal Energy = -648.681131
Enthalpy = -648.680187
Gibbs Free Energy = -648.736081

C,0,-1.7566784381,0.1779079004,-0.6384855512
C,0,-2.590740517,-1.0106250112,-0.3338184352
C,0,1.8716110741,0.4926037257,-0.895430756
C,0,0.4542362204,0.9135401122,-0.6385185061
O,0,0.1185415894,1.9725273984,-0.1819811418
O,0,-0.4073246076,-0.0650910493,-0.9564329712
C,0,-2.2187313825,-0.0302459347,0.7608141632
O,0,-3.1552391319,0.8827096055,1.2289123339
O,0,-3.8723691402,-1.0050343308,-0.8708130091
C,0,2.3963260292,-0.335177607,0.26961248
O,0,1.7257482634,-0.5182494558,1.2574182071
C,0,3.7785645793,-0.8903928448,0.1025882733
H,0,-2.2256639599,0.9839488514,-1.1864207826
H,0,-2.0839941301,-1.968094312,-0.3022340504
H,0,1.9465540955,-0.0965077329,-1.8090810237
H,0,2.5003867238,1.375335794,-1.0040114164
H,0,-1.4767453175,-0.3740763146,1.4727107777
H,0,-3.7697898162,0.4283892043,1.8141830456
H,0,-4.4693553398,-1.4427726176,-0.2556514666
H,0,3.7773823367,-1.6029272863,-0.7235743279
H,0,4.4706466727,-0.0913046842,-0.1630202635
H,0,4.0995331962,-1.3820204107,1.0155774209

TS–diOHCPr-3-Oxobutanoate

E (total electronic) = -648.8104362
E (total electronic) + ZPVE = -648.641302
Internal Thermal Energy = -648.627984
Enthalpy = -648.627039
Gibbs Free Energy = -648.684226

C,0,1.8192729202,-0.13363012,0.075147024
C,0,2.7589016357,-0.8499609373,-0.6653900286
C,0,2.1147116142,1.0668051782,-0.5715412932
O,0,2.287402991,2.1825499585,0.1379255306
O,0,3.5828382908,-1.699325877,-0.0465773773
H,0,1.9231829784,-0.1427968733,1.1509251918
H,0,2.7770859857,-0.8288271122,-1.7454205773
H,0,2.1034774076,1.1530358226,-1.6485214225
H,0,2.5821115197,2.90590584,-0.4269926551
H,0,4.2459221484,-2.0411541792,-0.6567855125
C,0,-2.145766779,-0.7075251685,0.7293294052
C,0,-0.7081618246,-0.2280997992,0.8452800158
O,0,-0.4131380298,0.6411544535,1.6613952008
O,0,0.1045388968,-0.7895781575,0.0222393527
C,0,-2.9006290963,0.0473829785,-0.3465098634
O,0,-2.417646381,0.9945490079,-0.9237588815

C,0,-4.2839313167,-0.4556449308,-0.6487930106
H,0,-2.1897283124,-1.772067933,0.4982410504
H,0,-2.6707455794,-0.5474103496,1.6724220187
H,0,-4.2049246856,-1.4384996541,-1.1163780086
H,0,-4.8486743346,-0.5839166061,0.2742297594
H,0,-4.7984590494,0.2277744589,-1.3175049189

diOHCPr-Methyl Oxalate
1. dissociation
E (total electronic) = -684.7814555
E (total electronic) + ZPVE = -684.632602
Internal Thermal Energy = -684.619754
Enthalpy = -684.618809
Gibbs Free Energy = -684.673680

C,0,-1.7836722443,-0.0857741682,-0.5252565312
C,0,-2.8870826643,-0.838158645,0.1164681695
C,0,0.4832229445,0.3608887642,-0.3982883655
O,0,0.3261448765,1.5081174761,-0.695829005
O,0,-0.4728557218,-0.5511899787,-0.2845515435
C,0,-2.5422373447,0.564681848,0.5785688736
O,0,-3.3348182589,1.6408485375,0.2043136347
O,0,-4.0048626142,-1.0600682818,-0.6765699705
C,0,1.8567503531,-0.266303281,-0.0942154267
O,0,2.002215726,-1.4138789134,0.2192032576
O,0,2.8093222256,0.6299000621,-0.227892136
C,0,4.1418559591,0.1595683766,0.0324496963
H,0,-1.9554507358,0.2994933163,-1.5210285928
H,0,-2.605301191,-1.6363200756,0.7932616597
H,0,-2.0485935592,0.6353216877,1.5410138012
H,0,-4.1419827462,1.6337124347,0.7289748747
H,0,-4.7895172895,-1.0484271343,-0.1190862785
H,0,4.388472331,-0.6428482001,-0.6582474636
H,0,4.7892638409,1.0141219469,-0.1209700129
H,0,4.2099981134,-0.2001477719,1.0560153591

TS–diOHCPr-Methyl Oxalate
1. dissociation
E (total electronic) = -684.7331201
E (total electronic) + ZPVE = -684.586339
Internal Thermal Energy = -684.573549
Enthalpy = -684.572605
Gibbs Free Energy = -684.628624

C,0,-2.3741910542,-0.4977273739,-0.3189189863
C,0,-3.5132348617,-1.2232192657,0.0363539982
C,0,-2.9078925369,0.6494604798,0.2744108497
O,0,-2.9056479044,1.8068261511,-0.3945451185
O,0,-4.1249149476,-1.98339577,-0.8792011431
H,0,-2.1473734583,-0.4298059072,-1.3741233844
H,0,-3.8470331393,-1.3019566752,1.0604405788
H,0,-3.2042334766,0.6695255988,1.312820285
H,0,-3.3926891875,2.4818451993,0.0913163125
H,0,-4.9502313887,-2.3393591894,-0.5316126411
C,0,0.2254866363,-0.5207778448,-0.2085251943
O,0,0.2348636773,0.4364196872,-0.9625765017
O,0,-0.7855103903,-1.1636463939,0.2310201595
C,0,1.5726320821,-1.0823746942,0.3336443615
O,0,1.6511861115,-1.9612320148,1.1495293896
O,0,2.6106370908,-0.4722986947,-0.2137195355
C,0,3.8973714778,-0.9247262962,0.2261920188
H,0,4.6222168723,-0.330456585,-0.3176447199
H,0,3.9990981257,-0.7694326093,1.297748636
H,0,4.0175442717,-1.9812718021,-0.0018503647

diOHCPr-Oxalate, 2. dissociation
E (total electronic) = -645.0396448
E (total electronic) + ZPVE = -644.931958
Internal Thermal Energy = -644.921036
Enthalpy = -644.920092
Gibbs Free Energy = -644.970513

C,0,-0.4896294901,-0.8736264853,-0.0709584662
C,0,-0.0734182202,-1.6443665045,-1.2677975977
C,0,-0.3743604887,1.2186261652,0.9468147463
O,0,-0.2621936825,0.6887947142,2.0204464958
O,0,-0.5122518519,0.5258342666,-0.1968835026
C,0,0.8157149165,-1.5900665683,-0.0410847997
O,0,0.8868485679,-2.6800022372,0.818381118
O,0,-0.8147998829,-2.7876611343,-1.5443823017
C,0,-0.388718936,2.7621463666,0.7100666328
O,0,0.3145301701,3.4063397186,1.5035160352
O,0,-1.1072727302,3.1567060847,-0.2217308994
H,0,-1.2772878765,-1.2996825692,0.5360741338
H,0,0.267707026,-1.0725283751,-2.1229095911
H,0,1.7112884807,-0.9860513131,-0.1309502329
H,0,1.4295286005,-3.363691315,0.4127655207
H,0,-0.2322536026,-3.451003814,-1.9276452913

TS–diOHCPr-Oxalate, 2. dissociation
E (total electronic) = -644.9824109
E (total electronic) + ZPVE = -644.876794
Internal Thermal Energy = -644.865699
Enthalpy = -644.864755
Gibbs Free Energy = -644.916418

C,0,-1.2094045745,-2.0513027244,0.6448640593
C,0,-2.3600278088,-2.5944336437,1.2151133982
C,0,-1.3383977987,-2.7802998313,-0.5370226358
O,0,-0.2733927023,-3.3827306953,-1.0665959966
O,0,-2.3418253951,-3.0060254889,2.4843598547
H,0,-0.2817156898,-2.1648213365,1.187663787
H,0,-3.3094014467,-2.5990069542,0.6993656049
H,0,-2.2559110988,-2.7886770627,-1.1080646551
H,0,-0.5246174502,-3.9213795619,-1.825407641
H,0,-3.1675129225,-3.4463396491,2.7155399703
C,0,-0.0015611212,0.3111324302,0.4023972491
O,0,1.0491909581,-0.3180646983,0.2641251303
O,0,-1.1687377486,-0.2099261817,0.5597896605
C,0,0.0152426625,1.8507127243,0.3957162674
O,0,-0.1313148575,2.392724759,-0.7203353978
O,0,0.1836489941,2.3984869143,1.5059023445

diOHCPr-Methyl Malonate

1. dissociation

E (total electronic) = -724.105200
E (total electronic) + ZPVE = -723.927659
Internal Thermal Energy = -723.913593
Enthalpy = -723.912649
Gibbs Free Energy = -723.970693

C,0,1.7153353705,0.2371783457,-0.1830177925
C,0,2.7304797329,1.044559558,0.5354517951
C,0,-1.6375264313,-0.8971134081,0.7308134796
C,0,-0.2851529451,-0.9264608757,0.0726617387
O,0,0.0981985997,-1.7848276483,-0.6737517658
O,0,0.4408073476,0.1486765078,0.409063757
C,0,2.8667459499,-0.4629808302,0.4498852999
O,0,3.7789621905,-1.0349397871,-0.4272147677
O,0,3.5223426728,1.8653651664,-0.2581317102
C,0,-2.5796991049,-0.0165032145,-0.057896411
O,0,-2.3085440811,0.5124700263,-1.1050007
O,0,-3.7537890101,0.0879646966,0.5502944403
C,0,-4.738652389,0.8864252845,-0.1211313997
H,0,1.719501768,0.2868088374,-1.2635102913
H,0,2.4468766576,1.4368837599,1.5050668041
H,0,-2.0472420906,-1.9044723956,0.7594854477
H,0,-1.5685133436,-0.5169650629,1.7481216086
H,0,2.667811032,-1.0075817327,1.3657918958
H,0,4.6646629326,-0.9438422248,-0.0613984878
H,0,4.4028243118,1.9159798953,0.1275332433
H,0,-4.954385881,0.4645180063,-1.0996145987
H,0,-5.6189677486,0.8591532713,0.51010943
H,0,-4.3770975406,1.9056418246,-0.2322630155

TS–diOHCPr-Methyl Malonate
1. dissociation

E (total electronic) = -724.0513017
E (total electronic) + ZPVE = -723.875904
Internal Thermal Energy = -723.861848
Enthalpy = -723.860904
Gibbs Free Energy = -723.919876

C,0,2.1469595937,0.235019425,-0.0117251862
C,0,2.8465220598,1.3583553309,0.4293014561
C,0,3.1854684245,-0.6281594497,0.3406887665
O,0,3.587739942,-1.5698366834,-0.5146428065
O,0,2.8961728015,2.45197725,-0.3359958198
H,0,1.8378587096,0.2198987149,-1.0476882402
H,0,3.2597411927,1.4236814376,1.4252521583
H,0,3.606431124,-0.6396152641,1.3357220194
H,0,4.3711268209,-2.0232663235,-0.1831810333
H,0,3.4920744378,3.1081054175,0.0425040901
C,0,-1.6518662532,-1.0087882186,0.6697840972
C,0,-0.2326386196,-0.8926624244,0.1292731231
O,0,0.1327819311,-1.6172863784,-0.790880467
O,0,0.4796978335,0.006928166,0.7074442675
C,0,-2.5676647962,-0.0408767396,-0.0347355473
O,0,-2.2517829027,0.6845491338,-0.9437861949
O,0,-3.7995343857,-0.088369893,0.471303834
C,0,-4.7609040898,0.7819423541,-0.1370090216
H,0,-2.0355819165,-2.0147327392,0.5052196822
H,0,-1.6857279929,-0.7963857119,1.7368097858
H,0,-4.8706551834,0.5392244113,-1.1913511534
H,0,-5.6912747986,0.6108551557,0.3921720241
H,0,-4.4466221442,1.8177021807,-0.0324636392

diOHCPr-Malonate, 2. dissociation

E (total electronic) = -684.3559598
E (total electronic) + ZPVE = -684.219848
Internal Thermal Energy = -684.207674
Enthalpy = -684.206730
Gibbs Free Energy = -684.260349

C,0,-0.8960099906,-1.1423460162,0.1826487734
C,0,-0.732581011,-2.042347639,-0.986704657
C,0,-0.5319971101,2.4802050434,0.4002012475
C,0,-0.5361712575,1.0608971712,0.8596580454
O,0,-0.1558191053,0.6653426506,1.9322424058
O,0,-1.0055465,0.2296629789,-0.0937438028
C,0,0.4153896875,-1.8142358135,-0.0240843162
O,0,0.7508735011,-2.7927660958,0.9049616355
O,0,-1.4523198533,-3.2315588724,-0.943363402
C,0,0.7674528499,2.8031669748,-0.3948672233
O,0,1.6013089108,1.8825168201,-0.5126043636
O,0,0.8414902686,3.9680816461,-0.832345993
H,0,-1.4996726363,-1.508175824,1.0025688905
H,0,-0.6389229005,-1.5710487524,-1.958119428
H,0,-1.3855874303,2.6792503353,-0.2440833419
H,0,-0.5785726525,3.1374605907,1.2651690799
H,0,1.2241357823,-1.1906573617,-0.3877445463
H,0,1.2473136404,-3.4875955506,0.4609878518
H,0,-0.9273341934,-3.9279902856,-1.3503208558

TS–diOHCPr-Malonate, 2. dissociation

E (total electronic) = -684.295657
E (total electronic) + ZPVE = -684.161557
Internal Thermal Energy = -684.149299
Enthalpy = -684.148355
Gibbs Free Energy = -684.203492

C,0,1.7588944512,-0.5557436827,0.1078841151
C,0,2.688855671,-1.292619055,-0.6218273614
C,0,2.0199808599,0.6458243843,-0.5484364524
O,0,2.1502609852,1.773763733,0.1460509016
O,0,3.4915570072,-2.1548721516,0.0034805342
H,0,1.850702053,-0.5548202147,1.1843300674
H,0,2.7239281954,-1.2662731425,-1.7016094513
H,0,2.031630181,0.7164510782,-1.6268341246
H,0,2.4210960491,2.5005670286,-0.4264119683
H,0,4.1489070286,-2.5155032361,-0.6021745872
C,0,-2.229777196,-1.107024902,0.7579983258
C,0,-0.7940476834,-0.6415010887,0.860440969
O,0,-0.4797638472,0.2508137782,1.6528113253
O,0,0.0313043073,-1.2360660398,0.0688304701
C,0,-3.038187983,-0.3632884255,-0.333135742
O,0,-2.4800288262,0.5729159786,-0.9443509891

O,0,-4.2093077364,-0.7745212155,-0.4987970421
H,0,-2.2704525468,-2.1712939976,0.5324568309
H,0,-2.7337949698,-0.9380758292,1.7090971791

M06-2X/AUG-cc-pVDZ
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.7939529
E (total electronic) + ZPVE = -456.688413
Internal Thermal Energy = -456.680084
Enthalpy = -456.679140
Gibbs Free Energy = -456.721799

C,0,-0.8216984834,-0.2464188347,-0.3587143776
C,0,-2.0129283926,-0.8308138033,0.3149335618
C,0,1.4821380048,0.0282241001,-0.1615910071
O,0,1.4225867618,1.1509897673,-0.591975976
O,0,0.4326406221,-0.7898990604,-0.0004075817
C,0,-1.565787339,0.5877647474,0.6330487477
O,0,-2.2567988224,1.6715106527,0.0988236943
O,0,-3.1198501149,-1.046131935,-0.502022755
H,0,-0.9260788756,0.0369248549,-1.4045067636
H,0,-1.827244468,-1.5737010926,1.0918209249
H,0,-1.1021603497,0.7356299419,1.6093976235
H,0,-3.0807987649,1.782990366,0.5888418336
H,0,-3.9183185953,-0.9216157089,0.0256192157
H,0,2.405369297,-0.4796849953,0.1527032293

TS–diOHCPr-Formate
E (total electronic) = -456.7390676
E (total electronic) + ZPVE = -456.636094
Internal Thermal Energy = -456.627529
Enthalpy = -456.626585
Gibbs Free Energy = -456.670377

C,0,-1.2133780795,-0.0730316028,-0.0619595991
C,0,-2.3180445801,-0.8628689907,0.2843389599
C,0,-1.7295622522,1.0706244659,0.5635876807
O,0,-1.6865199418,2.2463754279,-0.0710879076
O,0,-2.8710704006,-1.659289314,-0.6382518335
H,0,-0.9787147309,0.0172821387,-1.1203460562
H,0,-2.6822319377,-0.9408878376,1.3062253756
H,0,-2.067454968,1.0637758304,1.5976064814
H,0,-2.1645617639,2.9191989466,0.431579621
H,0,-3.6804254486,-2.0617022425,-0.2966241284
C,0,1.4295298041,-0.1345131623,-0.0776311148
O,0,1.3881469971,0.8106962984,-0.8658412184
O,0,0.4250538176,-0.7329278687,0.4605404317
H,0,2.4124457344,-0.5503122294,0.233254358

diOHCPr-Acetate
E (total electronic) = -496.1029241
E (total electronic) + ZPVE = -495.970082
Internal Thermal Energy = -495.960012
Enthalpy = -495.959068
Gibbs Free Energy = -496.006187

C,0,-0.8199640851,-0.2548472407,-0.3534314146
C,0,-2.0182376253,-0.8334149127,0.3146452202
C,0,2.7629713369,-0.662149168,0.2695189269
C,0,1.4927811709,0.0102688362,-0.1564769308
O,0,1.3944720343,1.1311829301,-0.5977324132
O,0,0.425871218,-0.8056235266,0.0064619385
C,0,-1.5638114097,0.5816316284,0.6363777583
O,0,-2.2511538257,1.6693773021,0.1038374844
O,0,-3.1247272007,-1.0380314025,-0.5067650947
H,0,-0.9235924272,0.0304807524,-1.3988408603
H,0,-1.842572375,-1.5797182598,1.0905092345
H,0,2.6878575992,-0.9407562802,1.3266037636
H,0,2.9007256903,-1.5804684983,-0.3118847889
H,0,-1.1024767012,0.7260845978,1.6143647071
H,0,-3.0789022492,1.7768112074,0.5882119961
H,0,-3.9237679375,-0.880018072,0.0106903427
H,0,3.6030392769,0.0164580063,0.11400163

TS–diOHCPr-Acetate
E (total electronic) = -496.0445229
E (total electronic) + ZPVE = -495.913845
Internal Thermal Energy = -495.903655
Enthalpy = -495.902711
Gibbs Free Energy = -495.951374

C,0,-1.2203919773,-0.0180201838,-0.019291925
C,0,-2.3028052993,-0.8556584611,0.2784080983
C,0,-1.7830011359,1.112481056,0.5874386939
O,0,-1.7177065287,2.2952496538,-0.0303925429
O,0,-2.7674346307,-1.6889387905,-0.6585982977
H,0,-0.9287974995,0.0799654077,-1.0625866902
H,0,-2.7245554693,-0.9303600556,1.2782852712
H,0,-2.1847738044,1.0898637691,1.5983481108
H,0,-2.2263695504,2.958990702,0.4540092758
H,0,-3.5698588542,-2.1317484561,-0.3520422218
C,0,2.7779117766,-0.7321693625,0.3718846207
C,0,1.4440989186,-0.152630481,-0.0649316348
O,0,1.3826297001,0.6847539611,-0.9734949962
O,0,0.4213350063,-0.6174967617,0.5785560079
H,0,2.8727005271,-0.6716909536,1.4616039997
H,0,2.8112392962,-1.7925474551,0.0926695944
H,0,3.6017441446,-0.2003425187,-0.1110952141

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.698927
E (total electronic) + ZPVE = -574.509259
Internal Thermal Energy = -574.496521
Enthalpy = -574.495577
Gibbs Free Energy = -574.549335

C,0,-1.1285309435,-0.0038436343,-0.5142370872
C,0,-2.2459403733,-0.8971879534,-0.1007484259
C,0,2.4993374312,-0.4393983467,-0.1971677918
C,0,1.1818996145,0.2888900675,-0.3178734621
O,0,1.0169710278,1.4826784803,-0.2225537369
O,0,0.1588519646,-0.5753106747,-0.5134039542
C,0,-1.806637863,0.252690316,0.792203474

O,0,-2.5708812115,1.4150195293,0.8545696545
O,0,-3.4147072284,-0.7863191539,-0.8507590917
C,0,3.6708208324,0.5064167475,-0.4270150297
C,0,2.5580795063,-1.0963988798,1.1903006722
H,0,-1.3292939413,0.7087594906,-1.3121971908
H,0,-1.9800367662,-1.8978820459,0.2421887126
H,0,2.4955730283,-1.2312355404,-0.9567934001
H,0,-1.2618609212,-0.0235307875,1.6964531022
H,0,-3.3490345948,1.2426626377,1.3987745764
H,0,-4.1685374178,-0.9360814295,-0.2670863422
H,0,3.6775137184,1.2974774949,0.3322003805
H,0,4.6117212384,-0.0512475553,-0.3574383822
H,0,3.6154857793,0.9768244739,-1.4152285615
H,0,1.7256862858,-1.792855399,1.3374760755
H,0,3.4983333433,-1.6494308672,1.2926245748
H,0,2.5217624907,-0.3291299702,1.9743822338

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.639800
E (total electronic) + ZPVE = -574.452427
Internal Thermal Energy = -574.439672
Enthalpy = -574.438728
Gibbs Free Energy = -574.493950

C,0,-0.7983807473,-1.8339578749,-0.1474699261
C,0,-1.793640517,-2.4991387545,-0.8742611362
C,0,0.2652247977,-2.5332514871,-0.7321774755
O,0,1.2630473167,-2.9804496069,0.0347331691
O,0,-2.9019980242,-2.9092892615,-0.2493605388
C,0,-0.2063614928,2.1640156444,0.5038189331
C,0,-0.2077621411,0.6416087567,0.6527693088
O,0,0.3843234929,0.093874958,1.5909836607
O,0,-0.8294988661,0.0117980863,-0.2919385348
C,0,-0.0256269358,2.8717421482,1.8413507657
C,0,0.9032488096,2.5457989222,-0.4838141128
H,0,-0.8622222968,-1.8578223389,0.9377989135
H,0,-1.7497204628,-2.6131304056,-1.9552110445
H,0,0.3655674669,-2.6444003685,-1.8096848233
H,0,1.8715587582,-3.5236283248,-0.4836600324
H,0,-3.4516819349,-3.4355504799,-0.8448025207
H,0,-1.1720980258,2.4427827212,0.0630721893
H,0,-0.0538196655,3.9592531081,1.6976817693
H,0,-0.8163607424,2.5949904688,2.5491055977
H,0,0.9397158107,2.6037680488,2.2868967565
H,0,0.9148241396,3.6315138066,-0.6397076474
H,0,1.882449143,2.2469153451,-0.0858454471
H,0,0.7557261173,2.057239888,-1.4538168239

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9988281
E (total electronic) + ZPVE = -613.781309
Internal Thermal Energy = -613.767241
Enthalpy = -613.766296
Gibbs Free Energy = -613.822883

C,0,-1.3327787049,-0.1621369633,-0.4275170554
C,0,-2.4145027993,-0.8918852618,0.2898962137
C,0,2.3150762615,-0.1294559631,0.0790386714
C,0,0.9378890937,0.3789914841,-0.318239931
O,0,0.6803260259,1.4848309198,-0.7336602531
O,0,-0.0144646362,-0.5669420276,-0.1447121112
C,0,-2.1113352578,0.5605080133,0.6233688765
O,0,-2.9525869709,1.5690108205,0.1600313285
O,0,-3.5359621992,-1.2092095001,-0.4733878004
C,0,2.6394022316,-1.391856653,-0.7325760771
C,0,3.346374666,0.9610574809,-0.2022909178
C,0,2.2870090262,-0.4606460139,1.5793785767
H,0,-1.5269370797,0.1286859241,-1.4582526491
H,0,-2.1076683161,-1.6277401499,1.0342669689
H,0,-1.6116464467,0.7398828358,1.5766146999
H,0,-3.7577652699,1.567389956,0.6921237046
H,0,-4.3155260054,-1.162067535,0.0934744115
H,0,3.6451244837,-1.7379905745,-0.4647141558
H,0,1.9253487737,-2.1940336238,-0.5196185938
H,0,2.6236011035,-1.1811112172,-1.8092406567
H,0,3.1238720218,1.8699406569,0.3680571294
H,0,4.3400760826,0.5996814632,0.0879832649
H,0,3.3655968156,1.2190620693,-1.2675127327
H,0,3.2842690963,-0.7959109154,1.8890835551
H,0,2.0221226708,0.424315329,2.1716576507
H,0,1.5679636927,-1.2582467532,1.794464508

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9397351
E (total electronic) + ZPVE = -613.724152
Internal Thermal Energy = -613.710271
Enthalpy = -613.709327
Gibbs Free Energy = -613.765792

C,0,-1.9268861202,-0.2296274517,-0.5076229517
C,0,-2.9676253355,-1.0728521173,-0.0990604362
C,0,-2.5182950771,0.9414313571,-0.0170355636
O,0,-2.5022321363,2.051082174,-0.7593988152
O,0,-3.4067798362,-2.0255595916,-0.9278007488
H,0,-1.6535751529,-0.2366848319,-1.5600596397
H,0,-3.3761703141,-1.0496393963,0.9088145924
H,0,-2.9087113647,1.0140051985,0.9958620738
H,0,-3.0252050351,2.7476213157,-0.3407824021
H,0,-4.1873650179,-2.4616098442,-0.5612017138
C,0,2.1305047272,-0.6952811476,-0.1049646938
C,0,0.7387517814,-0.1973089133,-0.5432861511
O,0,0.6127142333,0.614312288,-1.468537872
O,0,-0.2503833948,-0.7098125783,0.1151215467
C,0,3.2255963625,0.0892165172,-0.8243865996
C,0,2.2310319157,-2.1827836533,-0.4706219094
C,0,2.2763799301,-0.525046513,1.4115736595
H,0,4.2100201713,-0.2790520491,-0.5068534352
H,0,3.1430659661,-0.0254283286,-1.9110794976
H,0,3.1621982205,1.1586830334,-0.5895313524
H,0,3.2169660309,-2.5691342504,-0.1799910868
H,0,1.4606957157,-2.7643680944,0.048117641
H,0,2.1121205049,-2.3286953165,-1.552510542
H,0,3.2679327845,-0.8744400597,1.7284559975
H,0,2.1780564634,0.5305272261,1.6982030854
H,0,1.5135699774,-1.1025069728,1.9442818143

diOHCPr-Fluoroacetate

E (total electronic) = -595.3188422
E (total electronic) + ZPVE = -595.192651
Internal Thermal Energy = -595.182047
Enthalpy = -595.181103
Gibbs Free Energy = -595.229929

C,0,0.2399610484,-0.9460943634,-0.1941133569
C,0,0.8764146983,-1.4916391321,1.0354304512
C,0,-0.8511900261,2.4339046756,-1.0432937952
C,0,-0.8533016129,0.9214240079,-1.0594931537
O,0,-1.6186116096,0.2313425162,-1.6800481633
O,0,0.1369078407,0.4602614647,-0.2783318117
C,0,-0.6118324616,-1.6837674896,0.7871581328
O,0,-1.0911101259,-2.9152303065,0.3505904315
O,0,1.7589118733,-2.5492323803,0.8327359828
F,0,-1.8588687467,2.899229516,-1.8607454238
H,0,0.4499450149,-1.4535469499,-1.1337229072
H,0,1.1401493822,-0.7772264539,1.8162980107
H,0,-1.0215043964,2.791951281,-0.0212235755
H,0,0.112076385,2.806206906,-1.410719114
H,0,-1.2806942405,-1.0910848505,1.4128232059
H,0,-1.0942641069,-3.5262254098,1.0976737791
H,0,1.7029490838,-3.1448200313,1.5900093074

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.266123
E (total electronic) + ZPVE = -595.142025
Internal Thermal Energy = -595.131370
Enthalpy = -595.130426
Gibbs Free Energy = -595.180874

C,0,0.0194318647,-1.3044614292,-0.1391028249
C,0,-1.0179340246,-1.8086675572,-0.9358133715
C,0,1.0073367137,-1.9331941329,-0.9109885754
O,0,1.9942465469,-2.6005889255,-0.3031089435
O,0,-2.0954000721,-2.3457754127,-0.3490556878
H,0,-0.0006586071,-1.5575523267,0.9187308065
H,0,-1.0387849508,-1.6800758969,-2.0154265623
H,0,1.0706244168,-1.8041272681,-1.9892021604
H,0,2.5369737397,-3.065547156,-0.9535381173
H,0,-2.6750397937,-2.7470386542,-1.0098612745
C,0,0.8708094323,2.4387270533,1.1116493374
C,0,0.8802867741,0.9198087639,0.9756856607
O,0,1.6106828988,0.2202721144,1.6721115834
O,0,0.0539861189,0.5123106498,0.0718331046
F,0,1.774804141,2.8591191448,2.0778026592
H,0,1.1490893049,2.8963915132,0.1553285651
H,0,-0.1300485034,2.77621652,1.4049708009

diOHCPr-Chloroacetate

E (total electronic) = -955.6901266
E (total electronic) + ZPVE = -955.565661
Internal Thermal Energy = -955.554767
Enthalpy = -955.553823
Gibbs Free Energy = -955.603983

C,0,-0.0785492138,-1.0441765211,0.335984557
C,0,-0.8310318699,-1.8250725839,-0.6831683806
C,0,0.557482456,2.5335691617,0.6053969797
C,0,0.8368091676,1.0546989241,0.7720398711
O,0,1.8094996984,0.5552813115,1.2717229872
O,0,-0.1995528342,0.3617893233,0.2672324243
C,0,0.6884096667,-1.7641554742,-0.7246338354
O,0,1.4420514931,-2.8468771392,-0.2813806849
O,0,-1.471138848,-2.9667200474,-0.208616003
Cl,0,1.8730377203,3.5349141995,1.2629452537
H,0,-0.022151744,-1.4567334399,1.3415060357
H,0,-1.3506881294,-1.2590515812,-1.4573139439
H,0,0.4451389651,2.7596836962,-0.4583817542
H,0,-0.368453182,2.7862109552,1.1286102647
H,0,1.119818929,-1.1611923635,-1.5248857259
H,0,1.4229306041,-3.533358681,-0.9594636567
H,0,-1.463302879,-3.6345407398,-0.9052903889

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.6379399
E (total electronic) + ZPVE = -955.515510
Internal Thermal Energy = -955.504590
Enthalpy = -955.503645
Gibbs Free Energy = -955.555105

C,0,0.0302104497,-1.3412825481,-0.2657171559
C,0,-1.0159998409,-1.8347064864,-1.0581029026
C,0,1.0057290521,-1.9777665134,-1.0474892976
O,0,1.9888585672,-2.6600655361,-0.4494710911
O,0,-2.0929981084,-2.3673170221,-0.4661169022
H,0,0.0147544778,-1.599835479,0.7909812197
H,0,-1.044136159,-1.6998865245,-2.1367742304
H,0,1.0641577728,-1.8430667643,-2.1252165599
H,0,2.521492347,-3.1281535365,-1.105955374
H,0,-2.679725682,-2.76178218,-1.1246981609
C,0,0.8779165983,2.3945914063,0.9804069316
C,0,0.9023042557,0.8685641441,0.8650498158
O,0,1.6162757354,0.1590010508,1.5647916069
O,0,0.0827992444,0.4700333725,-0.0503281379
Cl,0,2.0092735143,3.0359643266,2.2147434391
H,0,1.1534118857,2.8343940731,0.0188727294
H,0,-0.1287671101,2.719975217,1.25397107

diOHCPr-Bromoacetate

E (total electronic) = -3069.67908
E (total electronic)+ZPVE = -3069.555142
Internal Thermal Energy = -3069.544106
Enthalpy = -3069.543161
Gibbs Free Energy = -3069.594766

C,0,-0.1405575519,-1.0838656364,0.3381866963
C,0,-0.8911100518,-1.8626634183,-0.684032329
C,0,0.5007063648,2.4905391579,0.6048438322
C,0,0.7809214416,1.0129755018,0.7721173266
O,0,1.7530331828,0.5076551012,1.2671307136

O,0,-0.259882283,0.3224048905,0.2711012446
C,0,0.6285255747,-1.8025293643,-0.7215192285
O,0,1.3808269631,-2.886148274,-0.2782268452
O,0,-1.533277772,-3.0044478501,-0.2125898396
Br,0,1.9279625405,3.5892483715,1.3003480337
H,0,-0.0869645633,-1.4979202321,1.3432568365
H,0,-1.4085445764,-1.2951192936,-1.4585416994
H,0,0.3825290307,2.7194805769,-0.4569180746
H,0,-0.4171254112,2.7493183982,1.1376653824
H,0,1.0621683743,-1.1982085466,-1.5195432318
H,0,1.3669088521,-3.5698268076,-0.9592951605
H,0,-1.5275341151,-3.6699705752,-0.911478657

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.6270914
E (total electronic)+ZPVE = -3069.505286
Internal Thermal Energy = -3069.494182
Enthalpy = -3069.493238
Gibbs Free Energy = -3069.545852

C,0,0.0376966615,-1.3629749657,-0.3158979467
C,0,-1.0144303114,-1.8534806325,-1.102495575
C,0,1.0056494083,-2.0088833404,-1.0995382632
O,0,1.9861270125,-2.6963088768,-0.5028842101
O,0,-2.0915120649,-2.3784072405,-0.5037809848
H,0,0.0248387958,-1.6187130811,0.7416030355
H,0,-1.0468947315,-1.7217453555,-2.1814528755
H,0,1.0612919503,-1.877783166,-2.1778343732
H,0,2.5132411809,-3.1700528315,-1.1597465488
H,0,-2.683615801,-2.771601621,-1.1582414505
C,0,0.8761153736,2.3696125443,0.9302865488
C,0,0.9120508339,0.8444018993,0.8175404437
O,0,1.6214176711,0.1338011839,1.5202372302
O,0,0.1008266906,0.4465542854,-0.1062832981
Br,0,2.0768591899,3.0867621747,2.2831185881
H,0,1.1664693208,2.8149475475,-0.0234911255
H,0,-0.1326501806,2.6938494759,1.1942718051

diOHCPr-Dichloroacetate

E (total electronic) = -1415.2731304
E (total electronic)+ZPVE = -1415.157777
Internal Thermal Energy = -1415.145912
Enthalpy = -1415.144968
Gibbs Free Energy = -1415.198398

C,0,1.6540600134,-0.3207965989,-0.4869809938
C,0,2.7441101111,0.6910711693,-0.5333525558
C,0,-1.9616494534,0.2088371706,-0.4886040844
C,0,-0.6436841938,-0.5041582394,-0.1826177292
O,0,-0.5260403178,-1.476094696,0.5108287389
O,0,0.352744497,0.1491282332,-0.7875476306
C,0,2.2923128507,0.1037282715,0.7951089212
O,0,3.062671467,-0.8681407169,1.4246299201
O,0,3.9319144759,0.2617723438,-1.116657866
Cl,0,-2.0719206915,1.6055777225,0.6250871287
Cl,0,-3.3376843979,-0.8818563673,-0.2872340614
H,0,1.8766315987,-1.3250043486,-0.841730646
H,0,2.4513916484,1.7250861364,-0.719825272
H,0,-1.9693654843,0.6011182146,-1.5059892536
H,0,1.7168968976,0.7697462296,1.4403020548
H,0,3.8256080742,-0.43949049,1.8319207672
H,0,4.6678369048,0.6975059656,-0.6692944381

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.224948
E (total electronic)+ZPVE = -1415.111740
Internal Thermal Energy = -1415.099822
Enthalpy = -1415.098878
Gibbs Free Energy = -1415.153218

C,0,-1.5022968934,-0.0812733111,-0.4388213172
C,0,-2.3681402024,-0.951042896,0.2431071608
C,0,-1.7898893505,0.9279829541,0.4962905063
O,0,-2.1455501871,2.1432101061,0.0592826346
O,0,-3.2881088316,-1.6414389449,-0.4507149601
H,0,-1.754330583,0.1401883717,-1.4739998473
H,0,-2.2292014669,-1.2003388548,1.2921847595
H,0,-1.6103159668,0.7991319998,1.5609934888
H,0,-2.4107080408,2.7022254552,0.8009809581
H,0,-3.8780235107,-2.1137222832,0.1511513841
C,0,2.401787413,-0.5179189377,-0.0067327819
C,0,1.0757784855,0.1905430252,-0.3645232261
O,0,0.9567059597,1.4011950257,-0.2505081055
O,0,0.1771538909,-0.6597617181,-0.7141232023
H,0,2.5407175202,-1.4268535245,-0.5914535197
Cl,0,3.8154924203,0.5267091587,-0.26216116
Cl,0,2.2870679931,-1.014815946,1.7153426479

diOHCPr-Trifluoroacetate

E (total electronic) = -793.7803087
E (total electronic) + ZPVE = -793.670095
Internal Thermal Energy = -793.658149
Enthalpy = -793.657205
Gibbs Free Energy = -793.710285

C,0,-0.7814560064,-0.2192970504,-0.4494415843
C,0,-1.9589974176,-0.7914095607,0.2557255351
C,0,2.8077456257,-0.6486200165,0.1891731735
C,0,1.51244531,0.0653616157,-0.2514587589
O,0,1.4951322192,1.1896332342,-0.6633750434
O,0,0.4838465796,-0.758052665,-0.0990515973
C,0,-1.5054037672,0.6322227621,0.5422878011
O,0,-2.1986596268,1.707756774,-0.0012162156
O,0,-3.0749024125,-1.0220637274,-0.541291699
F,0,3.8532292512,0.1634901916,0.0610615653
F,0,3.0232000197,-1.739202954,-0.5571825049
F,0,2.7229274325,-1.0335451373,1.4687904018
H,0,-0.8914066684,0.0407136818,-1.5001306726
H,0,-1.7576584738,-1.5189673709,1.0430214059
H,0,-1.0249235003,0.7933578019,1.5084333477
H,0,-3.0231057217,1.8220534464,0.4878033516
H,0,-3.8666268433,-0.8889660255,-0.0054315061

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.7358354
E (total electronic) + ZPVE = -793.627542
Internal Thermal Energy = -793.615659
Enthalpy = -793.614715
Gibbs Free Energy = -793.668258

C,0,-1.116036971,-0.5387498446,-0.3596365191
C,0,-2.2809536779,-1.1695759825,0.1053607094
C,0,-1.4882159426,0.6228900926,0.3385765431
O,0,-1.4792254936,1.802541837,-0.2986874195
O,0,-3.0718011835,-1.8119045764,-0.7693195976
H,0,-1.0176148095,-0.4359530894,-1.4388180292
H,0,-2.4955855308,-1.2842036641,1.1647734272
H,0,-1.6477993508,0.6261326485,1.4139688081
H,0,-1.8579862456,2.4901485906,0.264497655
H,0,-3.8866126323,-2.0978305334,-0.3362349294
C,0,2.7931442912,-1.3116610936,0.1071178149
C,0,1.4636974072,-0.6286865144,-0.3131760912
O,0,1.5006806926,0.4780206522,-0.8239245658
O,0,0.4516880079,-1.3628596707,-0.0391920642
F,0,2.9411449525,-2.5017749999,-0.5016442441
F,0,3.8606193562,-0.5669422588,-0.1977925302
F,0,2.8191991299,-1.5356205932,1.4334590326

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.2782168
E (total electronic)+ZPVE = -1269.142918
Internal Thermal Energy = -1269.125323
Enthalpy = -1269.124379
Gibbs Free Energy = -1269.191150

C,0,2.4186979542,-0.5531625486,0.0853036536
C,0,3.2413864699,0.0497941284,-0.9961607519
C,0,2.8110303598,0.883967983,0.2016160523
O,0,3.7160653301,1.1622658139,1.2190787267
O,0,4.545035008,-0.4251572396,-1.0855678237
C,0,-1.197372836,-1.2163681317,0.2570340265
F,0,-1.1561791286,-2.3426719952,-0.4880182109
C,0,0.2224889611,-0.8720496988,0.7628124094
O,0,0.4534944755,-0.639703475,1.9145769626
O,0,1.0777979038,-0.8794292775,-0.2498496548
F,0,-1.9940966103,-1.4336728518,1.3169692208
C,0,-1.861478329,-0.1298049725,-0.6230081832
C,0,-1.9160129613,1.2719456315,0.0141362743
F,0,-3.1219022233,-0.5182675467,-0.8870196162
F,0,-1.1857549888,-0.0274392519,-1.7812294414
F,0,-2.6015675526,1.2475576155,1.1537194997
F,0,-2.4968958882,2.1223280724,-0.8261428235
F,0,-0.670841312,1.6938475388,0.2655168363
H,0,2.9006248287,-1.2539958297,0.7635679992
H,0,2.7338892468,0.2760449853,-1.934742555
H,0,2.0429007391,1.6335267502,0.0070356519
H,0,4.3215795412,1.849023108,0.9134872689
H,0,5.1118720116,0.2914841916,-1.3967955218

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.2351165
E (total electronic)+ZPVE = -1269.101626
Internal Thermal Energy = -1269.084192
Enthalpy = -1269.083247
Gibbs Free Energy = -1269.149211

C,0,1.0105256568,2.1352491669,-0.4527286589
F,0,-0.1195703685,2.810392646,-0.1271630336
C,0,0.8247979226,0.6080865876,-0.2194179937
O,0,1.7203443422,-0.0060954321,0.3347838683
O,0,-0.2795727556,0.1779297073,-0.7001961315
F,0,2.0093549633,2.6112778095,0.3205356407
C,0,1.3372123586,2.5156187808,-1.9144171374
C,0,2.4988380575,1.7234035013,-2.5446073476
F,0,1.6612956413,3.8245059544,-1.9579812747
F,0,0.2500753274,2.3196363909,-2.6839562309
F,0,3.5994087002,1.8243039393,-1.8008986955
F,0,2.7554397228,2.200051747,-3.7618361092
F,0,2.1657013299,0.4339125399,-2.6531799242
C,0,-0.3583769087,-1.6146262576,-0.7640809868
C,0,-1.3345168234,-2.1845177466,-1.5972626297
C,0,0.6163594468,-2.3705610752,-1.4396162159
O,0,1.488105275,-3.1010509097,-0.7283697043
O,0,-2.4363857187,-2.717626737,-1.0440704658
H,0,-0.4579646699,-1.80904751,0.3020988027
H,0,-1.3073549784,-2.0804087579,-2.6789129255
H,0,0.7821593541,-2.2789800789,-2.5101148445
H,0,2.0203514617,-3.6527206494,-1.3162314472
H,0,-2.9631213373,-3.1690126168,-1.7163245552

M06-2X/6-311+G(3df,2p) IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.8868989
E (total electronic) + ZPVE = -456.780871
Internal Thermal Energy = -456.772624
Enthalpy = -456.771680
Gibbs Free Energy = -456.814141

C,0,-0.8218469177,-0.2442961664,-0.3529603888
C,0,-2.0105199942,-0.8291877689,0.31409938
C,0,1.4784949634,0.0278630322,-0.1641432483
O,0,1.4261701519,1.1412558716,-0.5984954984
O,0,0.4305026127,-0.7801966231,0.0026872833
C,0,-1.5687939208,0.586579353,0.6323923478
O,0,-2.2580698086,1.6670563831,0.1031911727
O,0,-3.1120102205,-1.0498298375,-0.499694442
H,0,-0.9254513759,0.0360237665,-1.3930420568
H,0,-1.8237604187,-1.5665277633,1.0869918146
H,0,-1.1083994093,0.7325918335,1.6034606906
H,0,-3.0770740345,1.7871127447,0.5930339154
H,0,-3.9126244785,-0.9223748999,0.0178079432
H,0,2.3944533308,-0.4803009255,0.1506414567

TS–diOHCPr-Formate
E (total electronic) = -456.8317749
E (total electronic) + ZPVE = -456.728515
Internal Thermal Energy = -456.719966
Enthalpy = -456.719022
Gibbs Free Energy = -456.762861

C,0,-1.2108315276,-0.0773639598,-0.0714996931
C,0,-2.3123985503,-0.8573841826,0.2815702514
C,0,-1.72365728,1.0601517614,0.5540395045
O,0,-1.6981004482,2.2331928782,-0.0751773846
O,0,-2.8842967064,-1.6448164245,-0.6292948057
H,0,-0.984372397,0.0101217718,-1.1253135879
H,0,-2.657197475,-0.9368178936,1.3028145764
H,0,-2.0426746122,1.0497388699,1.586759067
H,0,-2.1732443632,2.9036682622,0.4272650019
H,0,-3.6918854631,-2.0404653437,-0.2847393299
C,0,1.4254650991,-0.1287280164,-0.0704668742
O,0,1.3921483866,0.8241743435,-0.8373038141
O,0,0.4233053095,-0.7376878951,0.442998249
H,0,2.4009522776,-0.5453643114,0.2437398893

diOHCPr-Acetate
E (total electronic) = -496.2047273
E (total electronic) + ZPVE = -496.071240
Internal Thermal Energy = -496.061264
Enthalpy = -496.060320
Gibbs Free Energy = -496.107226

C,0,-0.8191947558,-0.2529882046,-0.3482335948
C,0,-2.0139597104,-0.8310949763,0.3158773612
C,0,2.7564931177,-0.6626025544,0.2685943905
C,0,1.4899273925,0.0127650126,-0.1584116886
O,0,1.3974127189,1.1249859432,-0.6021148024
O,0,0.4255721133,-0.7948207424,0.0090964685
C,0,-1.565410758,0.5821429625,0.6339521874
O,0,-2.2517745987,1.6650907295,0.1042344544
O,0,-3.1158468287,-1.0438427635,-0.5006521178
H,0,-0.9233476791,0.0271956876,-1.3884912031
H,0,-1.8356783735,-1.5698965201,1.0893741448
H,0,2.6776476072,-0.9539700276,1.3148321697
H,0,2.8997442505,-1.5685887728,-0.3183602637
H,0,-1.1067098403,0.72739664,1.6060171915
H,0,-3.0748766105,1.7812275503,0.5879446708
H,0,-3.9165565927,-0.8861537785,0.0080480318
H,0,3.5950710376,0.0104217145,0.1283840999

TS–diOHCPr-Acetate
E (total electronic) = -496.146109
E (total electronic) + ZPVE = -496.014956
Internal Thermal Energy = -496.004831
Enthalpy = -496.003886
Gibbs Free Energy = -496.052190

C,0,-1.2186217386,-0.0288078465,-0.0361474009
C,0,-2.3012454699,-0.8531666885,0.2681292036
C,0,-1.7671697693,1.0928890906,0.5853567123
O,0,-1.7196835588,2.2774909789,-0.0187618662
O,0,-2.7987368466,-1.6645291953,-0.6635469727
H,0,-0.9439069376,0.0751876519,-1.076735458
H,0,-2.6951497826,-0.9377211014,1.2711860414
H,0,-2.1421582949,1.0600178706,1.59896401
H,0,-2.2182956102,2.9372721572,0.4749835338
H,0,-3.600203068,-2.0988955602,-0.3525476105
C,0,2.7732860504,-0.7200097711,0.3800598769
C,0,1.4407124651,-0.1532668011,-0.0758920502
O,0,1.3860711496,0.697680138,-0.9612488004
O,0,0.4200282836,-0.6439501888,0.5371609167
H,0,2.8781167963,-0.589788557,1.4562579165
H,0,2.7975872101,-1.790118916,0.1757100161
H,0,3.5953337415,-0.2305821912,-0.1341579185

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.8173774
E (total electronic) + ZPVE = -574.626969
Internal Thermal Energy = -574.614335
Enthalpy = -574.613391
Gibbs Free Energy = -574.666898

C,0,-1.1261054704,-0.0052940064,-0.5015278657
C,0,-2.2464807198,-0.8944615342,-0.1046970818
C,0,2.4965654827,-0.4423411614,-0.1966363505
C,0,1.1804466636,0.286711201,-0.3083479424
O,0,1.0212724708,1.4739318385,-0.2159109492
O,0,0.1583772922,-0.5708535719,-0.4937369747

C,0,-1.8164262312,0.249461713,0.7934550961
O,0,-2.5756986702,1.4087370496,0.8560860275
O,0,-3.4032237018,-0.785229988,-0.8637054309
C,0,3.6648119617,0.5026985159,-0.4341070966
C,0,2.5688290518,-1.0925573982,1.1918833355
H,0,-1.3191480866,0.7048711064,-1.2951388987
H,0,-1.9849094233,-1.8897372391,0.2373570311
H,0,2.4886523595,-1.232906192,-0.9490640791
H,0,-1.2834232085,-0.0305793493,1.6959960385
H,0,-3.3533891588,1.2452408495,1.3978754108
H,0,-4.1652093588,-0.926332086,-0.2940878943
H,0,3.6794431639,1.2868845344,0.3225506325
H,0,4.601695787,-0.0498475554,-0.3753077923
H,0,3.6021589338,0.9755246345,-1.4133682227
H,0,1.740205065,-1.7799096069,1.3541166562
H,0,3.5021718155,-1.6458413166,1.2864188904
H,0,2.545958982,-0.3266034375,1.9685684604

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.7581654
E (total electronic) + ZPVE = -574.570126
Internal Thermal Energy = -574.557415
Enthalpy = -574.556470
Gibbs Free Energy = -574.611718

C,0,0.1370402981,-1.8628981339,-0.1617757923
C,0,-1.0747253735,-2.5285614273,-0.3394396803
C,0,0.7302207165,-2.4094162329,-1.299395684
O,0,1.9767115491,-2.8693272891,-1.2457442932
O,0,-1.6736924463,-3.1051312588,0.7004604764
H,0,0.6556581216,-2.0047066054,0.7759661272
H,0,-1.6071702514,-2.5123242317,-1.2801470975
H,0,0.2450966678,-2.3851504596,-2.2653289005
H,0,2.2182227668,-3.3070348828,-2.0690422004
H,0,-2.4408175709,-3.614414379,0.4180087978
C,0,0.9894705559,2.0958144017,0.3756703666
C,0,1.0682382426,0.5686474503,0.3836326521
O,0,2.1002888851,-0.0063356659,0.7243163817
O,0,0.0029660627,-0.0224274494,-0.0317919782
C,0,1.3202968591,2.5795356115,-1.040008588
C,0,1.9250336642,2.7219078094,1.4000352
H,0,-0.0435478053,2.366531019,0.6008293988
H,0,0.6435788183,2.1454577218,-1.7754733823
H,0,1.2407123689,3.6654743571,-1.0972772862
H,0,2.3426641874,2.3010405924,-1.3030078224
H,0,1.8252116097,3.8079270425,1.3856620775
H,0,1.7061237972,2.3702719092,2.4083875726
H,0,2.9602362764,2.468621101,1.1724446547

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.1251958
E (total electronic) + ZPVE = -613.906979
Internal Thermal Energy = -613.893029
Enthalpy = -613.892085
Gibbs Free Energy = -613.948186

C,0,-1.3023754813,0.2051111485,-0.7644691186
C,0,-2.4783388701,-0.4293313305,-0.1181281981
C,0,2.3022621733,-0.0933145207,-0.1044184872
C,0,0.9960026022,0.5412480402,-0.5502902456
O,0,0.8624651792,1.6593231916,-0.9699075718
O,0,-0.0424555407,-0.3067558023,-0.4202021855
C,0,-2.0728455061,0.9869379566,0.2423416985
O,0,-2.7935045286,2.0641389996,-0.2527027288
O,0,-3.5743899614,-0.6506228335,-0.9403390102
C,0,2.5532683793,-1.3600455053,-0.9327540271
C,0,3.4362126511,0.9055270588,-0.311780283
C,0,2.1819094443,-0.4573285031,1.3818979855
H,0,-1.415549913,0.5127704424,-1.7959780912
H,0,-2.2769543611,-1.1855238802,0.6326294707
H,0,-1.6158963743,1.1162837587,1.2177066867
H,0,-3.6168210647,2.1433874214,0.2381657448
H,0,-4.3788714252,-0.5309813318,-0.4271447022
H,0,3.5038555407,-1.7992000462,-0.6282690508
H,0,1.7660953735,-2.095674901,-0.7773007185
H,0,2.610383078,-1.127621496,-1.9970358962
H,0,3.2704657652,1.8128562995,0.2681517311
H,0,4.3748741053,0.4542635087,0.0102462065
H,0,3.5270932655,1.1830682286,-1.3616284468
H,0,3.1264058239,-0.8849410018,1.7198684016
H,0,1.971843496,0.4265903728,1.9859042004
H,0,1.3922391492,-1.1888132749,1.5455726358

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.0659154
E (total electronic) + ZPVE = -613.849835
Internal Thermal Energy = -613.835996
Enthalpy = -613.835052
Gibbs Free Energy = -613.891553

C,0,-1.9274519347,-0.2492679389,-0.5272868147
C,0,-2.973320774,-1.0653785228,-0.0989845716
C,0,-2.4862796538,0.9229168238,-0.01915862
O,0,-2.4875143121,2.0323514001,-0.7519558641
O,0,-3.4668058564,-1.9940616443,-0.9156553079
H,0,-1.6826757673,-0.2575936846,-1.5802467781
H,0,-3.3416601063,-1.0422846274,0.9170974717
H,0,-2.8350700821,0.9936394961,1.001859809
H,0,-2.9886425317,2.7323181678,-0.3199501133
H,0,-4.2471498129,-2.4110648704,-0.5349950528
C,0,2.1261789791,-0.695436,-0.1107825174
C,0,0.7334003271,-0.2152497905,-0.564078523
O,0,0.6111398449,0.6165966568,-1.4612121177
O,0,-0.2512363366,-0.7625125986,0.0582487924
C,0,3.2195662007,0.0998252229,-0.8167001796
C,0,2.2548122087,-2.1811519297,-0.4670627095
C,0,2.251857504,-0.5193247282,1.40532753
H,0,4.1989805503,-0.2528377149,-0.4879342224
H,0,3.1543696708,-0.017506909,-1.8979049203
H,0,3.1411873442,1.1627884549,-0.587515068
H,0,3.2371148558,-2.5486904935,-0.1640079815
H,0,1.4924147709,-2.7700406324,0.0413655656
H,0,2.1524768423,-2.3350286736,-1.5430690589
H,0,3.237026159,-0.8555419481,1.7342209757
H,0,2.1399749679,0.5293678127,1.6878339028
H,0,1.4936829422,-1.0997833283,1.9282513737

diOHCPr-Fluoroacetate
E (total electronic) = -595.4424699
E (total electronic) + ZPVE = -595.315669
Internal Thermal Energy = -595.305163
Enthalpy = -595.304219
Gibbs Free Energy = -595.352808

C,0,0.2357749712,-0.9450785332,-0.1921982526
C,0,0.8728902633,-1.4877520923,1.0324342818
C,0,-0.8507266201,2.4286578153,-1.0426371204
C,0,-0.8539922193,0.9171740321,-1.0628502667
O,0,-1.6132625389,0.2347825083,-1.6850328054
O,0,0.1272290839,0.4554080717,-0.282112915
C,0,-0.6107220427,-1.6842818378,0.7854702274
O,0,-1.088673565,-2.9121489466,0.3542971259
O,0,1.7579721073,-2.5371453831,0.8350204687
F,0,-1.852162415,2.8992442127,-1.8458875513
H,0,0.4466743666,-1.4506603282,-1.1253606841
H,0,1.1313339964,-0.7743670916,1.8071342121
H,0,-1.0080805567,2.7784905423,-0.0222602696
H,0,0.1094357981,2.7953413295,-1.4056420672
H,0,-1.2760486909,-1.0944788062,1.4066705054
H,0,-1.0986837058,-3.5229537597,1.0972036336
H,0,1.7069797673,-3.1347787331,1.5867794774

TS–diOHCPr-Fluoroacetate
E (total electronic) = -595.3894591
E (total electronic) + ZPVE = -595.264838
Internal Thermal Energy = -595.254272
Enthalpy = -595.253328
Gibbs Free Energy = -595.303141

C,0,0.0061644313,-1.3057592881,-0.1218735738
C,0,-1.0130872435,-1.80566797,-0.9334562285
C,0,0.9972299639,-1.9186574434,-0.8911167644
O,0,1.9756686972,-2.5977315869,-0.2948767685
O,0,-2.0879558529,-2.3656190853,-0.376485475
H,0,-0.023749318,-1.5707533911,0.9261975278
H,0,-1.022619087,-1.6524912675,-2.0031927291
H,0,1.0690492051,-1.7645989352,-1.958671791
H,0,2.5234638072,-3.05215538,-0.9437259791
H,0,-2.6536302542,-2.7647572567,-1.0459203038
C,0,0.8790198505,2.43200897,1.1050055752
C,0,0.882973013,0.9125530953,0.9759459638
O,0,1.6342588152,0.2216067236,1.6450850244
O,0,0.0294075742,0.5045295985,0.1085881858
F,0,1.8038581125,2.8585946149,2.0313858832
H,0,1.1198224746,2.877889646,0.1401839292
H,0,-0.1094681891,2.7668259561,1.418942524

diOHCPr-Chloroacetate
E (total electronic) = -955.8029484
E (total electronic) + ZPVE = -955.677984
Internal Thermal Energy = -955.667146
Enthalpy = -955.666202
Gibbs Free Energy = -955.716279

C,0,-0.0740100365,-1.0423176997,0.331153963
C,0,-0.8280011748,-1.8211784687,-0.6813266137
C,0,0.5584077256,2.5290229046,0.606705021
C,0,0.8384975271,1.0518018813,0.7740205011
O,0,1.8041746796,0.5593882798,1.2765446441
O,0,-0.1876744341,0.3592455978,0.2658233306
C,0,0.6874535424,-1.7659589201,-0.7243865363
O,0,1.4381863359,-2.8457549153,-0.2856941564
O,0,-1.4728209615,-2.9548695988,-0.2096680075
Cl,0,1.8590416787,3.5299445678,1.2572580079
H,0,-0.0191669607,-1.4526550168,1.3309373505
H,0,-1.3418261759,-1.255794568,-1.4508793209
H,0,0.440144171,2.7511886419,-0.4506452024
H,0,-0.3659744489,2.7772959161,1.1214803871
H,0,1.1161175491,-1.1672893967,-1.5207892417
H,0,1.4254307167,-3.5313137071,-0.9601693323
H,0,-1.4676697338,-3.6264864978,-0.8980607939

TS–diOHCPr-Chloroacetate
E (total electronic) = -955.7503734
E (total electronic) + ZPVE = -955.627503
Internal Thermal Energy = -955.616632
Enthalpy = -955.615688
Gibbs Free Energy = -955.667077

C,0,0.0163255803,-1.3433529982,-0.2489198837
C,0,-1.0110856666,-1.8332126693,-1.0567384724
C,0,0.9961739321,-1.9635498249,-1.02716521
O,0,1.970915003,-2.6564366624,-0.4402041374
O,0,-2.0861151049,-2.3888168359,-0.4955173664
H,0,-0.0095760951,-1.6128237333,0.7982237251
H,0,-1.0267916022,-1.6743254444,-2.125551491
H,0,1.0638439212,-1.8043206853,-2.094191831
H,0,2.5096555323,-3.1134082179,-1.0947983857
H,0,-2.6584477647,-2.7809202803,-1.1634200664
C,0,0.885063179,2.388265818,0.9763407372
C,0,0.9025153743,0.8618521563,0.8648135491
O,0,1.6370009377,0.1611064893,1.5387495329
O,0,0.0563768169,0.4624969893,-0.0148734958
Cl,0,2.0440034867,3.0319104525,2.1619191571
H,0,1.1238806546,2.8202171787,0.0089319729
H,0,-0.1081811846,2.7139792679,1.2713486655

diOHCPr-Bromoacetate
E (total electronic) = -3069.7745719
E (total electronic)+ZPVE = -3069.650179
Internal Thermal Energy = -3069.639182
Enthalpy = -3069.638238
Gibbs Free Energy = -3069.689754

C,0,-0.1299304273,-1.0826469181,0.3324899788
C,0,-0.8919675453,-1.8609694678,-0.6743321947
C,0,0.504313605,2.4863935622,0.59903854
C,0,0.7846034084,1.0111952122,0.7748481213

O,0,1.7482749913,0.5142495741,1.2769195426
O,0,-0.2439049828,0.3190573557,0.2683284139
C,0,0.6232141216,-1.8055288252,-0.7293468655
O,0,1.3779213439,-2.8854984577,-0.2979034813
O,0,-1.5330751931,-2.9948080338,-0.1978874217
Br,0,1.8871554723,3.5925427263,1.353816451
H,0,-0.067412951,-1.4932548825,1.331696597
H,0,-1.4119858844,-1.2954230041,-1.4395847849
H,0,0.4288985269,2.7161559674,-0.4596628351
H,0,-0.4329544042,2.7401153845,1.0843685418
H,0,1.045097322,-1.2060168622,-1.5287257771
H,0,1.3638026131,-3.5684889675,-0.9749954241
H,0,-1.5334640164,-3.6661523635,-0.8865624019

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.7221752
E (total electronic)+ZPVE = -3069.599966
Internal Thermal Energy = -3069.588913
Enthalpy = -3069.587968
Gibbs Free Energy = -3069.640419

C,0,0.0256627668,-1.3661803543,-0.3003953189
C,0,-1.0095675942,-1.8526977339,-1.1004503478
C,0,0.9963880193,-1.9967308356,-1.0819208578
O,0,1.9691106306,-2.6947954166,-0.4975499256
O,0,-2.0846135924,-2.3992529345,-0.5304279001
H,0,0.003860307,-1.6321864453,0.7478113197
H,0,-1.0310544701,-1.6975988041,-2.1697176645
H,0,1.0595980509,-1.8420400274,-2.149855066
H,0,2.5010574768,-3.157988236,-1.1533100167
H,0,-2.6637746139,-2.7899156715,-1.1932345753
C,0,0.8809761528,2.3638322188,0.9252163962
C,0,0.9119140461,0.8380164152,0.8185290139
O,0,1.6393340552,0.1370265429,1.4990935467
O,0,0.0776810651,0.438294884,-0.0732889797
Br,0,2.1060985265,3.0888192891,2.2420286351
H,0,1.146052373,2.8023175129,-0.0312196736
H,0,-0.1152421996,2.6910575961,1.2041024143

diOHCPr-Dichloroacetate

E (total electronic) = -1415.3977566
E (total electronic)+ZPVE = -1415.281866
Internal Thermal Energy = -1415.270102
Enthalpy = -1415.269158
Gibbs Free Energy = -1415.322140

C,0,1.6773916722,-0.4514768402,-0.3534700856
C,0,2.7691233182,0.4544568094,-0.7860669261
C,0,-1.9297602928,0.0744292981,-0.4935490374
C,0,-0.6117226224,-0.4957208248,0.0278710721
O,0,-0.4905859635,-1.1532092609,1.0152231671
O,0,0.3751819441,-0.1134693714,-0.7772523266
C,0,2.3452462721,0.399923575,0.6695639966
O,0,3.1201393122,-0.2776760955,1.596860132
O,0,3.9377632598,-0.1679270894,-1.1955114197
Cl,0,-1.999769955,1.7712260861,0.0284792381
Cl,0,-3.2988714353,-0.8412884984,0.1091343606
H,0,1.8876423742,-1.512139923,-0.3208499557
H,0,2.4773179959,1.3470039115,-1.3283257777
H,0,-1.9525785019,0.0656769438,-1.5770737546
H,0,1.7891793899,1.25820581,1.032271135
H,0,3.8890879426,0.257899006,1.8141005982
H,0,4.6871592897,0.3839544637,-0.9526624164

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3490919
E (total electronic)+ZPVE = -1415.235528
Internal Thermal Energy = -1415.223669
Enthalpy = -1415.222725
Gibbs Free Energy = -1415.276854

C,0,-1.1727059117,-1.0004303392,0.4387495984
C,0,-2.0120553954,-1.5260151736,-0.5476843259
C,0,-0.0977944879,-1.7023462326,-0.1180417847
O,0,0.6752388815,-2.4548506851,0.6666422611
O,0,-3.1786885306,-2.0794491594,-0.1983202025
H,0,-1.4209840306,-1.241052799,1.4638438793
H,0,-1.8229181895,-1.369698696,-1.5999071556
H,0,0.2118361994,-1.5526131352,-1.1427135365
H,0,1.3067840874,-2.9585244812,0.142928167
H,0,-3.6006699809,-2.4954768066,-0.9571488123
C,0,0.0359377948,2.7345009009,0.0834545383
C,0,0.0418290396,1.2787306667,0.6013499085
O,0,1.0828625984,0.7242710108,0.8906513237
O,0,-1.1374407304,0.7847788525,0.6055848124
Cl,0,0.0942510735,2.6503076917,-1.695810994
Cl,0,1.3866575636,3.6755859768,0.7124749674
H,0,-0.8830899813,3.2423964085,0.3482993554

diOHCPr-Trifluoroacetate

E (total electronic) = -793.9510243
E (total electronic) + ZPVE = -793.840233
Internal Thermal Energy = -793.828361
Enthalpy = -793.827416
Gibbs Free Energy = -793.880404

C,0,-0.7798155687,-0.2138347296,-0.4443266042
C,0,-1.955489232,-0.7929416741,0.2478995349
C,0,2.8053524927,-0.6483280601,0.1909415965
C,0,1.5121195781,0.0661541109,-0.2598987138
O,0,1.4997934979,1.1794468222,-0.6806346759
O,0,0.4840010494,-0.7459018699,-0.0988743283
C,0,-1.5083565203,0.6258207492,0.5469274037
O,0,-2.1996890078,1.7024454975,0.0169846903
O,0,-3.0647145234,-1.0227663988,-0.5494251866
F,0,3.8486573873,0.1443251121,0.0296190881
F,0,3.0005516897,-1.755403237,-0.5176259259
F,0,2.7251123538,-0.987872066,1.4735349578
H,0,-0.8882801515,0.0521469705,-1.4871341839
H,0,-1.754168342,-1.5212765691,1.0256430369
H,0,-1.0325696338,0.7768788724,1.5099291638
H,0,-3.0175292142,1.8237958481,0.5088633191
H,0,-3.8595898553,-0.8882243783,-0.0247061725

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.9061727
E (total electronic) + ZPVE = -793.797384
Internal Thermal Energy = -793.785553
Enthalpy = -793.784609
Gibbs Free Energy = -793.838195

C,0,-1.1141395281,-0.5357610016,-0.3653458593
C,0,-2.2730375056,-1.166507366,0.0958976405
C,0,-1.486567324,0.6138400776,0.3399920038
O,0,-1.4874700239,1.7971206592,-0.2787733387
O,0,-3.0694316971,-1.7986656141,-0.7725900095
H,0,-1.0157134073,-0.4268835711,-1.4374628962
H,0,-2.4762377634,-1.2909861889,1.1495477826
H,0,-1.6361703809,0.6033661425,1.4100042092
H,0,-1.8636864624,2.478469147,0.2882551364
H,0,-3.8820389496,-2.08613168,-0.3435591358
C,0,2.7889322368,-1.3106944581,0.1109152283
C,0,1.460895549,-0.6292003176,-0.3221868318
O,0,1.5019970166,0.4686476776,-0.8344096846
O,0,0.4519669247,-1.3558913855,-0.0488079159
F,0,2.916815104,-2.516324314,-0.446432052
F,0,3.8509216016,-0.5929257468,-0.2314898224
F,0,2.8213066096,-1.4775010605,1.4357735456

diOHCPr-Trichloroacetate

E (total electronic) = -1874.9881889
E (total electronic)+ZPVE = -1874.882746
Internal Thermal Energy = -1874.869721
Enthalpy = -1874.868776
Gibbs Free Energy = -1874.925732

C,0,-0.9285158937,-0.0398757379,-0.6658055788
C,0,-2.1007112248,-0.6334444471,0.0204885624
C,0,2.6620861586,-0.472369969,0.0009587247
C,0,1.3631866371,0.2267550592,-0.4775616488
O,0,1.3293699497,1.3462114174,-0.8803188932
O,0,0.3320640791,-0.5912559179,-0.3472029347
C,0,-1.6406294715,0.7724865333,0.3592848084
O,0,-2.331346523,1.8700644933,-0.127098531
O,0,-3.2205436271,-0.8301939438,-0.7712183698
Cl,0,4.0426555759,0.5683109208,-0.2951250404
Cl,0,2.8632570252,-1.9993279599,-0.8648534868
Cl,0,2.494483738,-0.771997109,1.7387853703
H,0,-1.0468220987,0.2593996487,-1.6985476047
H,0,-1.8962286017,-1.3877624668,0.7722236546
H,0,-1.1519379405,0.8895196086,1.320950915
H,0,-3.1412975423,1.982147557,0.3797379442
H,0,-4.0085592404,-0.712059687,-0.2324748913

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1874.9426971
E (total electronic)+ZPVE = -1874.839533
Internal Thermal Energy = -1874.826419
Enthalpy = -1874.825475
Gibbs Free Energy = -1874.883175

C,0,-1.292510678,-0.3574892702,-0.5896397241
C,0,-2.4469989653,-1.0009802621,-0.1356161228
C,0,-1.6450209101,0.7679582082,0.1635066317
O,0,-1.6505708429,1.9730865186,-0.4109763201
O,0,-3.2579223109,-1.5970975229,-1.0158285483
H,0,-1.2085724485,-0.2088445126,-1.6581686204
H,0,-2.6376780193,-1.1617987973,0.9154704303
H,0,-1.7805217135,0.7184140447,1.2344786051
H,0,-2.0146325634,2.6343800283,0.1868491068
H,0,-4.0660175606,-1.8975121637,-0.5872227036
C,0,2.6251628697,-1.1233046272,-0.0900160699
C,0,1.2764440383,-0.4546851602,-0.555103964
O,0,1.302280105,0.6598615469,-1.0263228744
O,0,0.2704598441,-1.1983654356,-0.3263756942
Cl,0,4.0196976749,-0.2048235352,-0.6495137454
Cl,0,2.7322665666,-2.7789302419,-0.7067119803
Cl,0,2.6115679139,-1.1478738177,1.6863105936

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.5570454
E (total electronic)+ZPVE = -1269.420786
Internal Thermal Energy = -1269.403417
Enthalpy = -1269.402473
Gibbs Free Energy = -1269.468491

C,0,2.4135118227,-0.5503472126,0.0845050956
C,0,3.2338989228,0.0473398899,-0.9950694255
C,0,2.8042406853,0.8824613912,0.1971637942
O,0,3.7032001722,1.1699398343,1.2101675308
O,0,4.5329267702,-0.4238347373,-1.0881619971
C,0,-1.1972973903,-1.2199376288,0.2565752637
F,0,-1.1567514058,-2.337668742,-0.4835642962
C,0,0.2228341308,-0.876700072,0.7637094327
O,0,0.4502749394,-0.6482578806,1.9094321368
O,0,1.076426969,-0.8800044462,-0.2418774262
F,0,-1.9894597471,-1.4322142222,1.3082622083
C,0,-1.8541347003,-0.1287835071,-0.6260619012
C,0,-1.9017493367,1.2721979761,0.0179689086
F,0,-3.1068157846,-0.5085394875,-0.8909888912
F,0,-1.1789873607,-0.0280017087,-1.7732774486
F,0,-2.5882206134,1.2480186688,1.1458543214
F,0,-2.4676081505,2.1235223802,-0.816602997
F,0,-0.6627120624,1.6790481119,0.2749297351
H,0,2.8955582379,-1.2440463703,0.7599137772
H,0,2.7264675178,0.2690992439,-1.927488858
H,0,2.0373279802,1.6234527978,-0.0000743185
H,0,4.2989426601,1.8645710518,0.9136658844
H,0,5.1028867433,0.2887476692,-1.3926605294

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.5136217
E (total electronic)+ZPVE = -1269.379352
Internal Thermal Energy = -1269.362085
Enthalpy = -1269.361141
Gibbs Free Energy = -1269.426562

C,0,1.0065073061,2.1363315696,-0.4529074503
F,0,-0.1171730216,2.8057268231,-0.1348919508
C,0,0.8220638746,0.608685394,-0.2161639615
O,0,1.7157435587,0.0010381023,0.3323365357
O,0,-0.2772615583,0.1778691319,-0.6892068762
F,0,1.9973536331,2.6106784867,0.3140457517
C,0,1.3338374006,2.5073949477,-1.918137416
C,0,2.4994696921,1.7095532521,-2.5383126303
F,0,1.6544410982,3.8069748499,-1.9687987493
F,0,0.2560284456,2.3046491111,-2.682011411
F,0,3.5902048396,1.8176108593,-1.7983602326
F,0,2.7551637277,2.1726943399,-3.750752563
F,0,2.1681385866,0.4283360769,-2.6341484746
C,0,-0.3562968909,-1.6109015469,-0.7599693508
C,0,-1.3272811145,-2.1769115411,-1.5912922182
C,0,0.6118807563,-2.3582098668,-1.441615134
O,0,1.4847555929,-3.094550811,-0.7484244789
O,0,-2.4225441842,-2.7204469982,-1.0487473596
H,0,-0.4512294544,-1.8081496562,0.2996324994
H,0,-1.3015062839,-2.057986414,-2.664680736
H,0,0.7730202864,-2.2501213448,-2.5046081457
H,0,2.0153096604,-3.6402226053,-1.3381811393
H,0,-2.9475199511,-3.1703211603,-1.718752509

M06-2X/6-31+G(d)
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.7165654
E (total electronic) + ZPVE = -456.610287
Internal Thermal Energy = -456.602138
Enthalpy = -456.601194
Gibbs Free Energy = -456.643427

C,0,-0.8237049701,-0.2428426738,-0.3554463224
C,0,-2.0120799638,-0.8319085924,0.3153955986
C,0,1.4845433963,0.0265068556,-0.1634567014
O,0,1.4335313498,1.1468211659,-0.6043523904
O,0,0.4309592398,-0.7825505073,0.0038896834
C,0,-1.5713725613,0.5875505701,0.6342666294
O,0,-2.2605622027,1.6703949714,0.097565736
O,0,-3.1132850209,-1.0548741738,-0.5060701355
H,0,-0.9258395511,0.0354686597,-1.4009069323
H,0,-1.8257188728,-1.5753862844,1.088731531
H,0,-1.1098545158,0.7400737145,1.6086883389
H,0,-3.0747176974,1.8082779619,0.6063614112
H,0,-3.921842258,-0.9388297141,0.0169464387
H,0,2.401014108,-0.4829329532,0.1543574847

TS–diOHCPr-Formate
E (total electronic) = -456.6599859
E (total electronic) + ZPVE = -456.556623
Internal Thermal Energy = -456.548038
Enthalpy = -456.547094
Gibbs Free Energy = -456.591046

C,0,-1.2170288232,-0.0702242027,-0.0639787259
C,0,-2.3167013272,-0.8607020523,0.2858330223
C,0,-1.7320514331,1.0692295827,0.564113348
O,0,-1.7027470443,2.2432230313,-0.0734783922
O,0,-2.8777979587,-1.6488314357,-0.6378474821
H,0,-0.9876923043,0.0199613856,-1.121085129
H,0,-2.6705565049,-0.9517810801,1.3070663897
H,0,-2.0545510361,1.066720107,1.5998086003
H,0,-2.1819122656,2.922862769,0.4272298315
H,0,-3.6901619932,-2.0582365616,-0.2995305505
C,0,1.4394586351,-0.1383524269,-0.0751676803
O,0,1.4058359871,0.8058593677,-0.8667205935
O,0,0.4320918473,-0.73365649,0.4584983628
H,0,2.417026471,-0.5536521341,0.240650049

diOHCPr-Acetate
E (total electronic) = -496.0222886
E (total electronic) + ZPVE = -495.888521
Internal Thermal Energy = -495.878538
Enthalpy = -495.877594
Gibbs Free Energy = -495.924564

C,0,-0.8239553995,-0.2524045644,-0.3522294894
C,0,-2.0181879381,-0.8326445172,0.3177761137
C,0,2.7613206379,-0.6652354178,0.2701633567
C,0,1.4923245086,0.0126778872,-0.1570393914
O,0,1.3992028096,1.1334887465,-0.6026750846
O,0,0.4237113227,-0.7979607005,0.0075505852
C,0,-1.5688520769,0.5846437898,0.6334903475
O,0,-2.2528864686,1.6704475464,0.0945817551
O,0,-3.1200783999,-1.0493387787,-0.505591027
H,0,-0.9275495555,0.0245333494,-1.3981436777
H,0,-1.8400507225,-1.5761449867,1.0930385453
H,0,2.6835938165,-0.9659771565,1.318207803
H,0,2.9135730234,-1.5684562705,-0.3266335984
H,0,-1.1078410255,0.7371475897,1.6082590266
H,0,-3.0683496473,1.8102543668,0.6004602919
H,0,-3.9290275674,-0.9123887703,0.0115135304
H,0,3.6015651725,0.0146257867,0.137362413

TS–diOHCPr-Acetate
E (total electronic) = -495.9622154
E (total electronic) + ZPVE = -495.830650
Internal Thermal Energy = -495.820505
Enthalpy = -495.819561
Gibbs Free Energy = -495.867897

C,0,-1.2286557783,-0.021944611,-0.0288969356
C,0,-2.3091895459,-0.8560190687,0.272764617
C,0,-1.7795160595,1.1035293052,0.5916670694
O,0,-1.7249805224,2.2881278755,-0.0220875236
O,0,-2.7927996276,-1.671701701,-0.6689378803
H,0,-0.9483793455,0.0822922897,-1.0722297858
H,0,-2.7144862669,-0.9477902836,1.2747331298
H,0,-2.1610513589,1.080460723,1.6071278541
H,0,-2.2271880855,2.9585715344,0.4682357289
H,0,-3.5986281359,-2.1192800357,-0.3646193667
C,0,2.7857088798,-0.7266181926,0.3775150373
C,0,1.4490734331,-0.1573755345,-0.0719785683
O,0,1.3898379657,0.6897498614,-0.9733146038
O,0,0.4251194387,-0.637783694,0.5557601722
H,0,2.8968219884,-0.6065166601,1.4586413403
H,0,2.8148634247,-1.7987793035,0.1608376856
H,0,3.6094142157,-0.2292214344,-0.1364478205

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.61042
E (total electronic) + ZPVE = -574.419354
Internal Thermal Energy = -574.406700
Enthalpy = -574.405756
Gibbs Free Energy = -574.459452

C,0,-1.1178229838,-0.2673990139,-0.2652146893
C,0,-2.2728102504,-0.7959866524,0.5080004143
C,0,2.4942164276,-0.2446920378,0.4077887727
C,0,1.1635360328,0.2365703415,-0.1260097326
O,0,0.9820105091,1.2257646037,-0.7993250853
O,0,0.1630570586,-0.6081177049,0.2100987061
C,0,-1.9567902309,0.6909333794,0.5130170809

O,0,-2.719142907,1.5705003315,-0.2503543984
O,0,-3.3314222389,-1.2838814071,-0.2539470624
C,0,2.9357148114,-1.4797938819,-0.3946732789
C,0,3.5365123895,0.8665743335,0.3496211152
H,0,-1.2198200091,-0.2308425367,-1.3467295051
H,0,-2.0487312788,-1.3363134373,1.426378111
H,0,2.3271064167,-0.5502090818,1.447342237
H,0,-1.5343199622,1.0894706775,1.4342245525
H,0,-3.5575564302,1.7390773143,0.2070078964
H,0,-4.1597938498,-1.1263712189,0.2251640481
H,0,3.0776584483,-1.2199402362,-1.449374372
H,0,3.8888872768,-1.84709129,-0.0037203096
H,0,2.2007120137,-2.2859899512,-0.3285086179
H,0,3.2152017299,1.7477631623,0.9120760265
H,0,4.479100776,0.5095018971,0.774299018
H,0,3.718271251,1.1702534092,-0.6859269271

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.5498733
E (total electronic) + ZPVE = -574.360725
Internal Thermal Energy = -574.348091
Enthalpy = -574.347147
Gibbs Free Energy = -574.401639

C,0,0.2564016498,-1.1795765211,-0.3737230004
C,0,-0.4211742714,-1.9229702948,-1.3444946235
C,0,1.4333238367,-1.9302072759,-0.4516642881
O,0,2.0576069534,-2.2964436085,0.6700784887
O,0,-1.690790521,-2.2808099027,-1.1312585062
H,0,-0.2027151251,-1.0899846027,0.6056497772
H,0,0.0060804196,-2.1404591937,-2.317707101
H,0,1.9265591205,-2.145399691,-1.3936890254
H,0,2.8024861168,-2.887976151,0.4769343428
H,0,-2.0080008422,-2.8769419941,-1.8285194343
C,0,0.4802029453,2.8977835136,0.067263393
C,0,0.5444477378,1.3912775241,0.3338566393
O,0,0.7317798377,0.9582387301,1.4792456596
O,0,0.3470531537,0.6500533773,-0.7078510145
C,0,-0.9895829065,3.3365607643,0.1357540637
C,0,1.3357254474,3.6896310017,1.0516188571
H,0,0.8427237322,3.0617990484,-0.9538090943
H,0,-1.077586248,4.4055304167,-0.0845925311
H,0,-1.605118772,2.786266823,-0.5823835158
H,0,-1.3916422427,3.1636829237,1.1408300548
H,0,1.2921981798,4.7580699094,0.8148642488
H,0,0.9731703835,3.547998015,2.0743922391
H,0,2.3832804146,3.3734251881,1.0177833708

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9064292
E (total electronic) + ZPVE = -613.687130
Internal Thermal Energy = -613.673267
Enthalpy = -613.672323
Gibbs Free Energy = -613.728239

C,0,-1.3080397249,0.2096176329,-0.770808969
C,0,-2.4799889005,-0.4281811034,-0.1141581477
C,0,2.3045355845,-0.0927749421,-0.1050805316
C,0,0.9980913365,0.5447215568,-0.5549085007
O,0,0.8639296246,1.6704307244,-0.979314087
O,0,-0.0446266206,-0.3058030101,-0.4258091242
C,0,-2.0754453482,0.9931038847,0.2417486063
O,0,-2.7989264362,2.0707743076,-0.2610195808
O,0,-3.5795625743,-0.6552768644,-0.9378135392
C,0,2.5556876293,-1.3613873515,-0.9365846115
C,0,3.4435833252,0.9062780933,-0.3078129184
C,0,2.1784740376,-0.4601676481,1.3832559042
H,0,-1.4228063071,0.5138476064,-1.8079048421
H,0,-2.2738186092,-1.1882885102,0.6377623109
H,0,-1.6131350707,1.1322166433,1.2181862062
H,0,-3.622397764,2.1603063478,0.2435674861
H,0,-4.3883718624,-0.5692645673,-0.409557482
H,0,3.5084526823,-1.8060634739,-0.6305831956
H,0,1.7642649141,-2.0999298575,-0.7842435223
H,0,2.6161745912,-1.12842536,-2.005184385
H,0,3.2802853366,1.8172232145,0.2757571296
H,0,4.3847266132,0.4511990221,0.0169811734
H,0,3.5409115546,1.1877795063,-1.3607691821
H,0,3.1245474,-0.8913953763,1.7269131336
H,0,1.9661618206,0.4252518833,1.9924219966
H,0,1.3846657679,-1.1944403583,1.5450946725

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.8455593
E (total electronic) + ZPVE = -613.628443
Internal Thermal Energy = -613.614576
Enthalpy = -613.613632
Gibbs Free Energy = -613.670169

C,0,-1.9398506893,-0.2317557135,-0.515774871
C,0,-2.9784456724,-1.0714482487,-0.1040094415
C,0,-2.5183039466,0.9359766081,-0.0096094597
O,0,-2.5144697617,2.0478061596,-0.7473547455
O,0,-3.4377874861,-2.007002601,-0.9398630443
H,0,-1.6787017906,-0.2318395684,-1.569027715
H,0,-3.3691535781,-1.06523184,0.9080081175
H,0,-2.8870615253,1.0083510843,1.0083322536
H,0,-3.0307259747,2.7515349922,-0.3227001341
H,0,-4.2217437081,-2.4481619237,-0.5752936599
C,0,2.1344240729,-0.6955485338,-0.1079711025
C,0,0.7404059547,-0.2031495865,-0.5497638359
O,0,0.614913877,0.6240642086,-1.463403778
O,0,-0.2490859649,-0.732277328,0.0925188698
C,0,3.232093546,0.0872777558,-0.8281694993
C,0,2.2447192522,-2.1869270161,-0.4612350609
C,0,2.2766855968,-0.5162864874,1.4094964953
H,0,4.2153325795,-0.2748448335,-0.5058760498
H,0,3.1580047114,-0.0331942981,-1.9131288393
H,0,3.1685622202,1.1567855194,-0.6025655933
H,0,3.2304178203,-2.5665012559,-0.1674413608
H,0,1.4799060405,-2.7706291161,0.0594070371
H,0,2.1282987985,-2.3459772016,-1.5397284631
H,0,3.2655743079,-0.8617243513,1.7330218988
H,0,2.1768240729,0.5380724052,1.6931675463
H,0,1.5155432471,-1.0903208297,1.9446694352

diOHCPr-Fluoroacetate

E (total electronic) = -595.2248682
E (total electronic) + ZPVE = -595.097824
Internal Thermal Energy = -595.087350
Enthalpy = -595.086405
Gibbs Free Energy = -595.135002

C,0,0.2394514309,-0.9509721265,-0.1937601659
C,0,0.8771388286,-1.4911743039,1.0354651503
C,0,-0.8484076193,2.4342345374,-1.0400659789
C,0,-0.854586899,0.9196784171,-1.0613510326
O,0,-1.6217774572,0.2334448071,-1.6859858069
O,0,0.1327558129,0.4544154584,-0.2818887299
C,0,-0.6097700593,-1.6883559372,0.7870327128
O,0,-1.0892945481,-2.917408697,0.3462401542
O,0,1.7674438564,-2.5410768978,0.8314702139
F,0,-1.8573570954,2.900296705,-1.8540339733
H,0,0.4538198941,-1.4561504448,-1.1316051893
H,0,1.1404344739,-0.7755318492,1.8126544936
H,0,-1.0167176485,2.7932123937,-0.0215232593
H,0,0.1096646934,2.8088377968,-1.4090610819
H,0,-1.281606423,-1.0986060711,1.4089126382
H,0,-1.1380729431,-3.5245691795,1.10089801
H,0,1.7328197027,-3.1348216083,1.5976298455

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.1706894
E (total electronic) + ZPVE = -595.045850
Internal Thermal Energy = -595.035233
Enthalpy = -595.034289
Gibbs Free Energy = -595.084328

C,0,0.0079218848,-1.3150068556,-0.1291805474
C,0,-1.0183775919,-1.8106894258,-0.9406813997
C,0,1.0027443498,-1.9277053392,-0.9003169115
O,0,1.9810044446,-2.6079879209,-0.2945284926
O,0,-2.0941363743,-2.3679246688,-0.3716831772
H,0,-0.0213943803,-1.5813477457,0.9227743525
H,0,-1.0381729361,-1.6592617365,-2.0143734268
H,0,1.0831881543,-1.7763725922,-1.9715711125
H,0,2.5368292526,-3.0681446789,-0.9436820064
H,0,-2.6725235732,-2.7684160357,-1.0403262976
C,0,0.8752232409,2.4443866697,1.1076993736
C,0,0.8823937095,0.9225987841,0.9789292913
O,0,1.6354727925,0.2271960971,1.6572563201
O,0,0.0301738231,0.5105452229,0.1034008738
F,0,1.8092862416,2.868447348,2.0415794218
H,0,1.1220915459,2.8997866079,0.1454131724
H,0,-0.1113185837,2.7857132694,1.4313055664

diOHCPr-Chloroacetate

E (total electronic) = -955.5846382
E (total electronic) + ZPVE = -955.459083
Internal Thermal Energy = -955.448409
Enthalpy = -955.447464
Gibbs Free Energy = -955.497097

C,0,-0.0754166887,-1.0477375627,0.3347264135
C,0,-0.8311980683,-1.823030534,-0.6838057364
C,0,0.5564909313,2.5335178956,0.6055356409
C,0,0.8403485968,1.0539154159,0.7741785693
O,0,1.8140361985,0.5583406718,1.2787862553
O,0,-0.1907157153,0.3581992752,0.2677414154
C,0,0.6877037671,-1.7694873425,-0.724952895
O,0,1.4394789212,-2.851400893,-0.2787333193
O,0,-1.4802881553,-2.9577232287,-0.2066866146
Cl,0,1.8664505206,3.5406170157,1.2574381175
H,0,-0.0244275156,-1.4582173045,1.33954363
H,0,-1.349817777,-1.2552241017,-1.4546115336
H,0,0.4372991416,2.7591125787,-0.4550472641
H,0,-0.368809501,2.7852474233,1.125307182
H,0,1.1241538908,-1.169564771,-1.5221339917
H,0,1.452926613,-3.5313668713,-0.9701083886
H,0,-1.4879051596,-3.6309286665,-0.9048734805

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.5308382
E (total electronic) + ZPVE = -955.407599
Internal Thermal Energy = -955.396702
Enthalpy = -955.395758
Gibbs Free Energy = -955.447284

C,0,0.0241954983,-1.3512471016,-0.2601240049
C,0,-1.0156640554,-1.8358741803,-1.0613911578
C,0,1.0028829647,-1.9761945078,-1.0424185721
O,0,1.978640125,-2.6701112511,-0.4475111842
O,0,-2.0909213647,-2.3823392904,-0.4809200119
H,0,0.0029974644,-1.6187534158,0.7918761106
H,0,-1.0460435514,-1.6828065378,-2.1345888396
H,0,1.0746441026,-1.8242304498,-2.1141496074
H,0,2.521521353,-3.1365449452,-1.1031069362
H,0,-2.6806457992,-2.7763944438,-1.1433975487
C,0,0.881569521,2.4005642116,0.9813863629
C,0,0.9042368729,0.8720339147,0.8691490393
O,0,1.6327518741,0.1657384803,1.5596413627
O,0,0.0700864136,0.4698247507,-0.0291237479
Cl,0,2.0269053269,3.0488747483,2.1944645181
H,0,1.1378746761,2.8380644017,0.0163460578
H,0,-0.1194744218,2.7280566163,1.2628151592

diOHCPr-Bromoacetate

E (total electronic) = -3067.2132515
E (tot. electronic) + ZPVE = -3067.088270
Internal Thermal Energy = -3067.077450
Enthalpy = -3067.076506
Gibbs Free Energy = -3067.127087

C,0,-0.1250744795,-1.080167871,0.321888631
C,0,-0.894792033,-1.8654592836,-0.6775963404
C,0,0.5035370813,2.4944730218,0.602672432
C,0,0.7864403895,1.0181015207,0.7722753928
O,0,1.7529869709,0.5191432633,1.2870955918
O,0,-0.2394602963,0.3245128752,0.2500387608

C,0,0.623685571,-1.8116319494,-0.7410889791
O,0,1.3833722842,-2.8884167155,-0.2954565387
O,0,-1.5361872224,-2.9951223754,-0.1779826047
Br,0,1.880585435,3.5870638919,1.3861613652
H,0,-0.0600776624,-1.4850623972,1.3282677828
H,0,-1.4243277973,-1.3073378784,-1.4480339116
H,0,0.4407751666,2.7370355029,-0.4583681407
H,0,-0.442723183,2.7457338235,1.081470258
H,0,1.0470216153,-1.2197518442,-1.5512453006
H,0,1.3815745159,-3.5781060582,-0.9773424905
H,0,-1.5587503556,-3.6740855264,-0.8702509079

TS–diOHCPr-Bromoacetate

E (total electronic) = -3067.1592522
E (tot. electronic) + ZPVE = -3067.036566
Internal Thermal Energy = -3067.025548
Enthalpy = -3067.024603
Gibbs Free Energy = -3067.076674

C,0,0.0401037845,-1.3682059166,-0.3217065983
C,0,-1.0134134988,-1.8540889312,-1.1041095432
C,0,1.0051536155,-2.0148233294,-1.1031483779
O,0,1.9795610199,-2.7084239382,-0.5058270288
O,0,-2.0875542962,-2.3784152733,-0.5017929778
H,0,0.026651138,-1.6214377548,0.7340853455
H,0,-1.0543957224,-1.7196963461,-2.1795228246
H,0,1.068181027,-1.8818555635,-2.1778989751
H,0,2.5124611758,-3.1902444391,-1.1584485496
H,0,-2.6896576443,-2.7776503703,-1.1497990725
C,0,0.8749565859,2.3769718782,0.9350405122
C,0,0.9161687783,0.8525985439,0.8106955714
O,0,1.6343480908,0.1464850786,1.5118077309
O,0,0.1064786073,0.4532443696,-0.1116903517
Br,0,2.0615489704,3.0821184503,2.2976036781
H,0,1.1665719341,2.8333022939,-0.0103813424
H,0,-0.133682566,2.7000992479,1.1905038037

diOHCPr-Dichloroacetate

E (total electronic) = -1415.1418561
E (tot. electronic) + ZPVE = -1415.025804
Internal Thermal Energy = -1415.014032
Enthalpy = -1415.013088
Gibbs Free Energy = -1415.066204

C,0,1.6549234163,-0.3172694217,-0.4785648314
C,0,2.74280898,0.6939062677,-0.5298950975
C,0,-1.9639062414,0.2096884653,-0.488729215
C,0,-0.6465828326,-0.5086692612,-0.1833715806
O,0,-0.5338519566,-1.4927837334,0.4956986657
O,0,0.3525300465,0.1526489944,-0.7704508144
C,0,2.3003932525,0.1030598227,0.7993785102
O,0,3.0688059936,-0.8735680396,1.4222260499
O,0,3.9227140367,0.2653942626,-1.1282303754
Cl,0,-2.0692161807,1.6211056954,0.6012405628
Cl,0,-3.339294091,-0.876332164,-0.2810946751
H,0,1.873860554,-1.3176121641,-0.8411580995
H,0,2.4503104378,1.7264426645,-0.7135956661
H,0,-1.9701927234,0.5870730434,-1.50886558
H,0,1.7298866313,0.7642960906,1.4506328041
H,0,3.8219476502,-0.44797246,1.8609812198
H,0,4.6706970268,0.7086219375,-0.6981588774

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.0922858
E (tot. electronic) + ZPVE = -1414.978469
Internal Thermal Energy = -1414.966600
Enthalpy = -1414.965656
Gibbs Free Energy = -1415.019726

C,0,-1.5071836966,-0.0775483087,-0.4423846071
C,0,-2.35778787,-0.9501111589,0.2499078605
C,0,-1.7894511322,0.9321778085,0.4900826469
O,0,-2.1581036863,2.1423714203,0.0515492095
O,0,-3.2810407689,-1.6459631192,-0.4324350329
H,0,-1.7690627063,0.1366386916,-1.4742008566
H,0,-2.2044045415,-1.2029892858,1.293240263
H,0,-1.5924126018,0.8144025001,1.5503772786
H,0,-2.4226889805,2.7117371998,0.791329838
H,0,-3.8724174244,-2.1211605668,0.1726281592
C,0,2.3990118793,-0.5209869648,-0.0026909681
C,0,1.078165652,0.1958226687,-0.3724676327
O,0,0.9632229163,1.4075252666,-0.2533676705
O,0,0.1787586838,-0.6481410812,-0.7320624809
H,0,2.5457572721,-1.4117731465,-0.6079322631
Cl,0,3.8140293582,0.5265077486,-0.2148351681
Cl,0,2.2537462965,-1.0644899922,1.6995568444

diOHCPr-Trifluoroacetate

E (total electronic) = -793.6613859
E (total electronic) + ZPVE = -793.550572
Internal Thermal Energy = -793.538744
Enthalpy = -793.537800
Gibbs Free Energy = -793.590787

C,0,-0.7837047404,-0.2146026328,-0.4502363301
C,0,-1.9566788191,-0.793216651,0.2535300021
C,0,2.8064224289,-0.6504018302,0.1910652484
C,0,1.5144793157,0.0677203841,-0.2549869341
O,0,1.5031394747,1.1921660818,-0.6705031234
O,0,0.4831785094,-0.7498506962,-0.1028643383
C,0,-1.5093112633,0.6309133203,0.5429263252
O,0,-2.2013277106,1.706697843,0.0000384618
O,0,-3.0685119148,-1.0308462471,-0.5459320279
F,0,3.8550876106,0.1541551677,0.0536950281
F,0,3.0132013839,-1.7483652298,-0.5439889986
F,0,2.7190491704,-1.020764762,1.4733378287
H,0,-0.8938825113,0.0433887324,-1.499543782
H,0,-1.7525556902,-1.5226144279,1.0356948944
H,0,-1.029550696,0.7945604936,1.5068034506
H,0,-3.0146529451,1.8479099552,0.5096689714
H,0,-3.8689956027,-0.9123845012,-0.0109876766

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.615704

E (total electronic) + ZPVE = -793.506907
Internal Thermal Energy = -793.495058
Enthalpy = -793.494114
Gibbs Free Energy = -793.547567

C,0,-1.1234621405,-0.5402822418,-0.3793504757
C,0,-2.2775227366,-1.1711805687,0.1047365961
C,0,-1.4787902698,0.615782268,0.3318393594
O,0,-1.4858952929,1.7976388324,-0.3000178918
O,0,-3.0880269723,-1.802883653,-0.7586414818
H,0,-1.0458399841,-0.4335303122,-1.4575415302
H,0,-2.4681717066,-1.3014502077,1.1640335085
H,0,-1.6071674189,0.6175878669,1.4086660868
H,0,-1.8543117627,2.4908702942,0.2705727657
H,0,-3.9023738626,-2.0923092906,-0.31751929
C,0,2.7904659204,-1.3090788999,0.1162317512
C,0,1.4654904337,-0.6271080397,-0.32200101
O,0,1.5070507158,0.4942477792,-0.8025599786
O,0,0.4528946547,-1.3736371915,-0.0902075667
F,0,2.9441746172,-2.5024888209,-0.4804307151
F,0,3.8601502696,-0.5669317551,-0.1821030197
F,0,2.7996775357,-1.5212750598,1.4436208919

diOHCPr-Trichloroacetate
E (total electronic) = -1874.6939161
E (tot. electronic) + ZPVE = -1874.588335
Internal Thermal Energy = -1874.575400
Enthalpy = -1874.574456
Gibbs Free Energy = -1874.630757

C,0,-0.9333923327,-0.052358789,-0.6634717443
C,0,-2.1018041077,-0.6255240915,0.0529248912
C,0,2.66698592,-0.480562999,0.000802594
C,0,1.3629890156,0.2279958518,-0.458756143
O,0,1.3275587131,1.3555126455,-0.8635567902
O,0,0.3312132612,-0.5964374499,-0.3284275016
C,0,-1.6431336714,0.7958582167,0.3384422285
O,0,-2.3356720654,1.8762308458,-0.1948428353
O,0,-3.2248894287,-0.85573179,-0.7331733042
Cl,0,4.0383453086,0.6136443026,-0.1905016121
Cl,0,2.9076643446,-1.935865881,-0.9930111301
Cl,0,2.484127589,-0.9308228691,1.7131793164
H,0,-1.0541986594,0.2077597139,-1.7112007815
H,0,-1.8926396355,-1.3570387848,0.8318079345
H,0,-1.1504481278,0.9559815268,1.2967239775
H,0,-3.1443046187,2.0189426818,0.321718417
H,0,-4.0178905048,-0.7409751307,-0.1864345167

TS–diOHCPr-Trichloroacetate
E (total electronic) = -1874.6476676
E (tot. electronic) + ZPVE = -1874.544440
Internal Thermal Energy = -1874.531299
Enthalpy = -1874.530355
Gibbs Free Energy = -1874.588487

C,0,-1.2991052834,-0.3585807818,-0.5895301073
C,0,-2.4530166026,-1.0035025531,-0.1243351869
C,0,-1.6454283817,0.7753942148,0.1606674594
O,0,-1.6503710661,1.9776768839,-0.4310813545
O,0,-3.2659711665,-1.6046699449,-1.0067261747
H,0,-1.2228909524,-0.2160014181,-1.6636617046
H,0,-2.6438990236,-1.1662811016,0.9304209354
H,0,-1.7732616229,0.7415422133,1.237153558
H,0,-2.0144988355,2.6524216495,0.1638744319
H,0,-4.0805520031,-1.9068370664,-0.5747183561
C,0,2.6316367457,-1.1255031593,-0.0871125116
C,0,1.282613766,-0.4550963978,-0.5555901884
O,0,1.3077409258,0.6673072235,-1.0294056557
O,0,0.2727613063,-1.2047878013,-0.3295266355
Cl,0,4.0343657513,-0.1773629467,-0.6118452168
Cl,0,2.7552181337,-2.7734997638,-0.75113546
Cl,0,2.6020913089,-1.20022425,1.6976711674

diOHCPr-Heptafluorobutanoate
E (total electronic) = -1269.0999063
E(tot. electronic) + ZPVE = -1268.963633
Internal Thermal Energy = -1268.946285
Enthalpy = -1268.945341
Gibbs Free Energy = -1269.011064

C,0,2.4271912279,-0.554235865,0.0842632893
C,0,3.244123244,0.0453458608,-1.0012165586
C,0,2.8260418164,0.8792716541,0.200040527
O,0,3.7338935664,1.1507427413,1.215843743
O,0,4.5420875938,-0.4408572726,-1.101495481
C,0,-1.1925599562,-1.2082864666,0.2613745912
F,0,-1.149386625,-2.3348875733,-0.480523539
C,0,0.2281955184,-0.8668200006,0.7681884795
O,0,0.459185261,-0.6383026875,1.9221642087
O,0,1.0831942976,-0.8740319542,-0.242628683
F,0,-1.9890120718,-1.4210988997,1.3211531231
C,0,-1.8576557853,-0.1254722954,-0.6235738407
C,0,-1.9468719482,1.2745293669,0.01715941
F,0,-3.1053740227,-0.5324764353,-0.9124447263
F,0,-1.1611440641,-0.0083888198,-1.7668183207
F,0,-2.6657370891,1.2379628309,1.1342146736
F,0,-2.5096037256,2.1214535817,-0.8365879735
F,0,-0.7149792512,1.7054715198,0.3079737028
H,0,2.9082259008,-1.2603625764,0.7547661269
H,0,2.7331576164,0.2724923863,-1.9355405519
H,0,2.0609645795,1.6315879143,0.0145989037
H,0,4.3222732334,1.8665716877,0.9288980666
H,0,5.1185516835,0.2698543025,-1.4234891708

TS–diOHCPr-Heptafluorobutanoate
E (total electronic) = -1269.0556042
E (tot. electronic) + ZPVE = -1268.921427
Internal Thermal Energy = -1268.904037
Enthalpy = -1268.903093
Gibbs Free Energy = -1268.968971

C,0,1.0178764569,2.1313951221,-0.4528303729
F,0,-0.1088886794,2.8054520242,-0.1199291601

C,0,0.830915161,0.6041414891,-0.2165082231
O,0,1.7310750171,-0.0105594086,0.3324099496
O,0,-0.2765931634,0.1744871313,-0.6886285587
F,0,2.022360443,2.6043095596,0.313399116
C,0,1.3346991029,2.5166355648,-1.9160512183
C,0,2.5045011307,1.7419508652,-2.5562249175
F,0,1.6397659194,3.8288002252,-1.9586204591
F,0,0.2465787518,2.3058656849,-2.6783644281
F,0,3.6082376514,1.8620482683,-1.8223238057
F,0,2.74218703,2.2193039845,-3.7752818295
F,0,2.1905810649,0.4483091249,-2.6573466773
C,0,-0.3636621007,-1.6234769078,-0.7589891844
C,0,-1.3339519813,-2.1826703972,-1.6021111394
C,0,0.6115246872,-2.3802279396,-1.4278522819
O,0,1.4698191526,-3.120993972,-0.7121114872
O,0,-2.44117518,-2.7143952798,-1.0600033143
H,0,-0.4746064962,-1.8198774535,0.3035060242
H,0,-1.3043389955,-2.0675308343,-2.6798054024
H,0,0.7960756557,-2.2783566003,-2.4917873896
H,0,2.0114868237,-3.6778177071,-1.2936570897
H,0,-2.9713614518,-3.1670715442,-1.7348361511

B3LYP/AUG-cc-pVTZ
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -457.0711702
E (total electronic) + ZPVE = -456.967293
Internal Thermal Energy = -456.958865
Enthalpy = -456.957921
Gibbs Free Energy = -457.000928

C,0,-0.8168743371,-0.1968735513,-0.295473577
C,0,-2.0189778281,-0.8206370505,0.3160922732
C,0,1.5287247721,-0.0000788998,-0.2197892893
O,0,1.5270364183,1.0550504652,-0.7982429291
O,0,0.4455366455,-0.7261444108,0.0889085507
C,0,-1.6185162033,0.6072524936,0.6767902665
O,0,-2.2977326652,1.7059428831,0.1470207298
O,0,-3.0832590574,-1.0797568568,-0.5506861078
H,0,-0.8857635326,0.0936463459,-1.334420884
H,0,-1.8508611816,-1.558280862,1.0934297176
H,0,-1.2076722837,0.7373609091,1.6721893263
H,0,-3.1262304989,1.8214097044,0.6266181902
H,0,-3.9091084173,-1.0122674423,-0.0577715253
H,0,2.4247686493,-0.5208547279,0.131305628

TS–diOHCPr-Formate
E (total electronic) = -457.0355404
E (total electronic) + ZPVE = -456.934063
Internal Thermal Energy = -456.925459
Enthalpy = -456.924514
Gibbs Free Energy = -456.969368

C,0,-1.1524524066,0.0207545677,0.006768494
C,0,-2.2470078625,-0.8189460578,0.2828983204
C,0,-1.7992375525,1.1066375471,0.6253491439
O,0,-1.8601477361,2.2947466142,-0.0086601403
O,0,-2.7637778246,-1.5831700249,-0.7004718171
H,0,-0.9146986681,0.1568710658,-1.0393876942
H,0,-2.5968024755,-0.9944672158,1.2889615298
H,0,-2.1136200292,1.0742361863,1.6575645302
H,0,-2.4262673122,2.9067517586,0.477205618
H,0,-3.5776344899,-2.0083662344,-0.4040529177
C,0,1.4490128691,-0.2481941931,-0.1396555781
O,0,1.4661226372,0.316996346,-1.2255323055
O,0,0.4158974773,-0.4921778613,0.6077644362
H,0,2.3838256236,-0.6192526383,0.3166394306

diOHCPr-2-Methylpropanoate
E (total electronic) = -575.0668619
E (total electronic) + ZPVE = -574.879118
Internal Thermal Energy = -574.866286
Enthalpy = -574.865341
Gibbs Free Energy = -574.919707

C,0,-1.1396021246,0.066354397,-0.3929049388
C,0,-2.3000008305,-0.8505322891,-0.2418943451
C,0,2.5046773513,-0.4582120579,-0.1273670573
C,0,1.2014755309,0.3107782083,-0.1958525162
O,0,1.0773935429,1.5075946366,-0.0826319974
O,0,0.1486735645,-0.5226340106,-0.3779559871
C,0,-1.9483660849,0.1431967054,0.8618654621
O,0,-2.6875132709,1.3146829056,1.0443214444
O,0,-3.3768324566,-0.6268514018,-1.104472593
C,0,3.6789798389,0.3930393837,-0.6069545147
C,0,2.7126163016,-0.9603208655,1.313727277
H,0,-1.2541516906,0.8891620183,-1.0850368015
H,0,-2.0838716026,-1.8894234901,-0.0166124982
H,0,2.3951488837,-1.3284673609,-0.7757801645
H,0,-1.5183396095,-0.2901875867,1.7584861611
H,0,-3.5038185045,1.099301683,1.5098790685
H,0,-4.1911399545,-0.8863113982,-0.658554168
H,0,3.8125696051,1.2682632558,0.0283529103
H,0,4.5959878546,-0.195059027,-0.5748139979
H,0,3.5311234578,0.7364023204,-1.6308231391
H,0,1.8846253523,-1.5868727873,1.6432335209
H,0,3.6273525249,-1.5502352884,1.3654851337
H,0,2.8095873207,-0.1221009511,2.004974741

TS–diOHCPr-2-Methylpropanoate
E (total electronic) = -575.0278615
E (total electronic) + ZPVE = -574.842107
Internal Thermal Energy = -574.829336
Enthalpy = -574.828391
Gibbs Free Energy = -574.884456

C,0,1.5032255864,-0.0187007242,-0.0073161916
C,0,2.4295400396,-0.9296857655,-0.5436114207
C,0,2.3062124055,1.0902044009,-0.3259896898
O,0,2.5223694551,2.0441387237,0.5996566602
O,0,2.7715651527,-2.0252956448,0.1608927305
H,0,1.2645899393,-0.1455755818,1.0400055329
H,0,2.7809062069,-0.8608546754,-1.562187419
H,0,2.6495960599,1.2824332226,-1.3315277232
H,0,3.1791256858,2.6772759638,0.2854387389
H,0,3.4957593028,-2.4934370407,-0.2721839845
C,0,-2.5084686154,-0.0881887873,-0.4770616195
C,0,-1.1273425341,-0.1513339563,0.1826877364
O,0,-1.0015613771,-0.2560131689,1.4025641175
O,0,-0.1367112602,-0.0513542945,-0.6638381397
C,0,-3.4840020861,-1.0810843185,0.1558831574
C,0,-3.0371923618,1.3523427004,-0.392843499
H,0,-2.3726075985,-0.3403862583,-1.5294034646
H,0,-4.4489018889,-1.0324804554,-0.3509182272
H,0,-3.1157374358,-2.1052446305,0.0817824377
H,0,-3.6406328778,-0.8540638826,1.210277745
H,0,-4.0016291235,1.4281161861,-0.896661377
H,0,-3.1745224691,1.6533302135,0.6469179878
H,0,-2.3530950782,2.0574688849,-0.8661733132

diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -614.3931816
E (total electronic) + ZPVE = -614.177846

Internal Thermal Energy = -614.163757
Enthalpy = -614.162813
Gibbs Free Energy = -614.219180

C,0,-1.3451078529,-0.0864929978,-0.3535428731
C,0,-2.442441189,-0.8975152924,0.2370706763
C,0,2.3376243983,-0.1203836074,0.0811154644
C,0,0.9607036504,0.4183625237,-0.3056085434
O,0,0.7355094854,1.4999841673,-0.7955994657
O,0,-0.0211540821,-0.4756813627,-0.0391505217
C,0,-2.2137679477,0.5425325533,0.6877473499
O,0,-3.0434281308,1.5784816366,0.2511036906
O,0,-3.4926776243,-1.2308944689,-0.6231040462
C,0,2.6101336879,-1.4183491255,-0.7050335342
C,0,3.4017902692,0.9284828403,-0.2584757253
C,0,2.3526814042,-0.4122975498,1.5949979687
H,0,-1.4878767515,0.2629310621,-1.3668644326
H,0,-2.1629190161,-1.6588027669,0.9574809396
H,0,-1.7948906701,0.6580077775,1.6816705651
H,0,-3.8642062973,1.5550901628,0.7563798858
H,0,-4.3067846494,-1.2913470672,-0.1104062971
H,0,3.6048414072,-1.7880393038,-0.4538607312
H,0,1.8853175299,-2.1925344879,-0.4606194433
H,0,2.5781759803,-1.2424165483,-1.7811647103
H,0,3.2315825097,1.8577262576,0.2841117128
H,0,4.3854306914,0.5474474135,0.0167954054
H,0,3.409750078,1.1560227521,-1.3238901802
H,0,3.3428760219,-0.7675308189,1.8821901914
H,0,2.1371617438,0.4874852195,2.17288882
H,0,1.6245537129,-1.1761451675,1.8614844597

TS–diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -614.3538576
E (total electronic) + ZPVE = -614.140702
Internal Thermal Energy = -614.126605
Enthalpy = -614.125661
Gibbs Free Energy = -614.183315

C,0,2.0420249962,0.1001546908,-0.2581127619
C,0,2.9303321012,1.1200292047,0.1237796901
C,0,2.8017167346,-0.9015301843,0.3705030405
O,0,3.0729155245,-2.0442254691,-0.2865346324
O,0,3.3348575627,2.0273840126,-0.7847924288
H,0,1.8912662992,-0.0291514825,-1.321088043
H,0,3.2045862083,1.287818802,1.1545314413
H,0,3.0664734435,-0.8510127205,1.4160646302
H,0,3.6917925404,-2.5859917333,0.218131136
H,0,4.0296314078,2.5872256082,-0.4172840924
C,0,-2.0089093196,0.1509360838,-0.0895014533
C,0,-0.5662227736,-0.1627157622,-0.5545242638
O,0,-0.3377874487,-0.8076710473,-1.577422004
O,0,0.3566202576,0.3260635401,0.228238981
C,0,-3.0240212699,-0.5388948744,-1.0065026859
C,0,-2.2160603149,1.6763877002,-0.1450033811
C,0,-2.1970986892,-0.3445741579,1.3553766991
H,0,-4.037012312,-0.3115695372,-0.6696175688
H,0,-2.9238590047,-0.200423214,-2.0370945303
H,0,-2.8972622934,-1.6213269452,-0.996039244
H,0,-3.2333196104,1.9229620931,0.1645229858
H,0,-1.5221162607,2.1931222951,0.5161447654
H,0,-2.072886923,2.0571170564,-1.1579915812
H,0,-3.2158646216,-0.1366357608,1.6874741763
H,0,-2.0352424877,-1.421793874,1.4270224017
H,0,-1.5065927468,0.1500566757,2.0360637235

diOHCPr-Fluoroacetate
E (total electronic) = -595.678726
E (total electronic) + ZPVE = -595.554343
Internal Thermal Energy = -595.543682
Enthalpy = -595.542737
Gibbs Free Energy = -595.591933

C,0,0.180669928,-0.9571861638,-0.1654553355
C,0,0.8787963975,-1.5027373176,1.0276122625
C,0,-0.8421459325,2.4525656082,-1.0525278327
C,0,-0.8552811408,0.9380962978,-1.108373647
O,0,-1.5627522971,0.2715654256,-1.8164732939
O,0,0.0558984092,0.4559872546,-0.24686012
C,0,-0.6192221926,-1.7261728164,0.8349952627
O,0,-1.1205646715,-2.9537242831,0.3988298882
O,0,1.8045751134,-2.519412932,0.7834479577
F,0,-1.7803887853,2.9661800293,-1.9314617131
H,0,0.3676657378,-1.4455879661,-1.1116873433
H,0,1.1430605823,-0.7990055105,1.8096386234
H,0,-1.0820330702,2.7883157465,-0.0437591123
H,0,0.1436542598,2.8248267221,-1.3310319212
H,0,-1.2615695982,-1.1594477556,1.5003848836
H,0,-1.1458747084,-3.5633918231,1.1452444689
H,0,1.8314499685,-3.1054175163,1.5485049724

TS–diOHCPr-Fluoroacetate
E (total electronic) = -595.6446435
E (total electronic) + ZPVE = -595.522236
Internal Thermal Energy = -595.511566
Enthalpy = -595.510622
Gibbs Free Energy = -595.560985

C,0,0.6881002509,-1.3497827333,-0.2108955557
C,0,-0.4238665101,-2.0759509755,-0.676647527
C,0,1.553380529,-2.2286881175,-0.8896065758
O,0,2.6041144401,-2.7654715951,-0.2358066131
O,0,-1.3804535813,-2.4592214642,0.1940490982
C,0,1.1430944653,2.6047378135,-0.1283271194
C,0,1.1847328204,1.1555579715,0.3486470577
O,0,1.5831563646,0.8463872469,1.4613506006
O,0,0.7465409897,0.3540698563,-0.5795274815
F,0,1.6210760063,3.4750371589,0.8495500344
H,0,0.8113418823,-1.3148643743,0.8631335233
H,0,-0.6265511964,-2.2014753033,-1.7295107923
H,0,1.5076088523,-2.364981657,-1.9594964709
H,0,3.0346353166,-3.4336449018,-0.7828469986
H,0,-2.0108924436,-3.0484763003,-0.2375678495
H,0,1.7612112913,2.7186807397,-1.0181765581
H,0,0.1169075225,2.8859066357,-0.3629247723

diOHCPr-Dichloroacetate

E (total electronic) = -1415.6561238
E (total electronic)+ZPVE = -1415.542693
Internal Thermal Energy = -1415.530567
Enthalpy = -1415.529623
Gibbs Free Energy = -1415.585510

C,0,-1.2793349739,-0.2078594702,-0.3029487161
C,0,-2.5064668817,-0.7886025737,0.2995636973
C,0,2.3318354806,-0.8404085427,0.2351254656
C,0,1.0638733137,-0.110281853,-0.2006715075
O,0,1.1110017793,0.9698575461,-0.729878031
O,0,-0.0402541386,-0.8043211734,0.0652564706
C,0,-2.0388657785,0.6123945108,0.688266833
O,0,-2.6602118504,1.7539463663,0.1813484465
O,0,-3.5784203715,-0.9850030121,-0.5723063832
H,0,-1.332905358,0.1048310358,-1.3362555317
H,0,-2.3696690262,-1.546586726,1.0633199239
H,0,-1.6215264262,0.6996205825,1.6856561282
H,0,-3.474099659,1.9107733591,0.673979418
H,0,-4.4016445131,-0.8987202502,-0.0780274531
Cl,0,2.5182859807,-2.3776309514,-0.6692853413
Cl,0,2.3337969342,-1.108789808,2.0076881311
H,0,3.1884307687,-0.2243674998,0.00173184

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.6250031
E (total electronic)+ZPVE = -1415.513566
Internal Thermal Energy = -1415.501428
Enthalpy = -1415.500484
Gibbs Free Energy = -1415.556279

C,0,-1.2730598786,0.1183748706,0.0496018835
C,0,-2.0884993967,0.9836730239,-0.7052072554
C,0,-2.0292234106,-0.9644823948,-0.4423427437
O,0,-2.5307120403,-1.8718354937,0.4225560259
O,0,-2.6520923133,2.0544514608,-0.1053399524
H,0,-1.3130096544,0.2564135402,1.1217066085
H,0,-2.1392719085,0.9282881524,-1.7818197131
H,0,-2.0719068196,-1.1994120046,-1.4949096172
H,0,-3.1222182428,-2.4804344217,-0.0364285932
H,0,-3.2821428136,2.4784830454,-0.7002861125
C,0,2.7066310043,-0.1764829154,0.4120229754
C,0,1.1963305001,-0.2601156384,0.7156343173
O,0,0.8596792734,-0.7452863737,1.785087057
O,0,0.4369215734,0.199458495,-0.2213288333
Cl,0,3.2231673814,1.5226135645,0.1353155438
Cl,0,3.1267060948,-1.2191208102,-0.9923920194
H,0,3.2712556512,-0.5443831004,1.2568334286

diOHCPr-Trifluoroacetate

E (total electronic) = -794.2414352
E (total electronic) + ZPVE = -794.133271
Internal Thermal Energy = -794.121257
Enthalpy = -794.120313
Gibbs Free Energy = -794.173695

C,0,-0.7795726359,-0.1514082676,-0.3859859281
C,0,-1.9708169407,-0.7895608909,0.2292122823
C,0,2.8395098001,-0.6661114672,0.1786534994
C,0,1.5567741625,0.0615327645,-0.3081155054
O,0,1.5824014223,1.1228677401,-0.8624638966
O,0,0.4953187551,-0.6773251669,-0.0151308453
C,0,-1.5747323975,0.6375272454,0.6025220527
O,0,-2.2547770418,1.7403214952,0.0875401656
O,0,-3.0343989709,-1.0492346738,-0.6349435787
F,0,3.9210464261,0.0620873428,-0.0990655208
F,0,2.9695452648,-1.860454104,-0.4219073121
F,0,2.7978900047,-0.8706975988,1.5054000088
H,0,-0.8488721227,0.1462102299,-1.4225175267
H,0,-1.790053198,-1.531237925,0.999795716
H,0,-1.1571899086,0.7545586083,1.5967176199
H,0,-3.0774223471,1.8566995884,0.577109687
H,0,-3.8592642723,-0.9913099204,-0.1391039179

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -794.2131885
E (total electronic) + ZPVE = -794.107041
Internal Thermal Energy = -794.095000
Enthalpy = -794.094056
Gibbs Free Energy = -794.148690

C,0,-1.0542389049,-0.4527382911,-0.2779430942
C,0,-2.2257781068,-1.148191902,0.0827503263
C,0,-1.581640846,0.6489869833,0.4280600194
O,0,-1.6478483793,1.8547326361,-0.1785197411
O,0,-2.9482673029,-1.7690418581,-0.8766342986
H,0,-0.9164359392,-0.2943336284,-1.3391796424
H,0,-2.4634668156,-1.3707123608,1.1116453604
H,0,-1.7480207894,0.6146955359,1.4938515644
H,0,-2.1368484331,2.4783830546,0.3716738478
H,0,-3.7820588132,-2.0894880764,-0.5121206756
C,0,2.8048302139,-1.3693682299,0.0983863939
C,0,1.5115180503,-0.6410781933,-0.389602186
O,0,1.5985737343,0.2807258661,-1.1749925697
O,0,0.4621390812,-1.1616336296,0.1494166468
F,0,2.7829827808,-2.6735319878,-0.2424725122
F,0,3.9084625046,-0.8305120938,-0.4340445222
F,0,2.9244399652,-1.3029228251,1.4390530828

diOHCPr-Trichloroacetate

E (total electronic) = -1875.2693381
E (total electronic)+ZPVE = -1875.166654
Internal Thermal Energy = -1875.153251
Enthalpy = -1875.152307
Gibbs Free Energy = -1875.209394

C,0,-0.9250781725,0.0208530571,-0.5901956369
C,0,-2.1186788201,-0.6258456754,0.0114076102
C,0,2.7038994997,-0.4922617742,-0.0201374966
C,0,1.4083321556,0.2323717679,-0.4931948913
O,0,1.4092337641,1.3092264077,-1.0170396096
O,0,0.3449570399,-0.5182319836,-0.2288831505

C,0,-1.720013508,0.7934217188,0.411394861
O,0,-2.3982252416,1.9065887064,-0.0842145356
O,0,-3.1830893258,-0.8674281228,-0.8574283593
Cl,0,4.1310022204,0.4909992274,-0.4096217396
Cl,0,2.82794792,-2.0784523492,-0.8469601449
Cl,0,2.6088339002,-0.7315078668,1.7559643511
H,0,-0.9940535424,0.3387916699,-1.6208211547
H,0,-1.9403864365,-1.3820627418,0.7682983701
H,0,-1.3041277492,0.8919854949,1.408265077
H,0,-3.223068064,2.0127635023,0.4038285558
H,0,-4.0069746401,-0.8246030387,-0.3584391056

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1875.2407042
E (total electronic)+ZPVE = -1875.139928
Internal Thermal Energy = -1875.126566
Enthalpy = -1875.125621
Gibbs Free Energy = -1875.184118

C,0,-0.4215827353,-1.4161558485,-0.3902962862
C,0,-0.6486863621,-2.0084722602,-1.6487766293
C,0,0.7488861645,-2.1997481418,-0.3103467047
O,0,0.9675636203,-2.9551231763,0.7883662676
O,0,-1.8504061552,-2.5705202542,-1.9080611671
H,0,-1.1672073831,-1.6287301073,0.3642001829
H,0,0.0257883943,-1.8639591873,-2.4787307533
H,0,1.5685067744,-2.0708467991,-1.0005279229
H,0,1.7335428233,-3.5260166508,0.6537290897
H,0,-1.8223058371,-3.0468432484,-2.7465277922
C,0,-0.325527,2.4026903005,0.7909996189
C,0,-0.4210837109,0.8286201253,0.858975273
O,0,-0.5315170077,0.2720662792,1.9304446595
O,0,-0.3598216614,0.3054184993,-0.3174006568
Cl,0,-0.4436790496,3.1307560239,2.4153926988
Cl,0,-1.6644065783,3.0344073813,-0.2280946955
Cl,0,1.2536607039,2.8582490642,0.0615548176

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.9989244
E (total electronic)+ZPVE = -1269.866834
Internal Thermal Energy = -1269.849037
Enthalpy = -1269.848092
Gibbs Free Energy = -1269.916047

C,0,2.7049961236,0.1998167356,-0.2886917682
C,0,3.6429408328,1.0836301196,0.4494731094
C,0,3.7915290234,-0.4350368987,0.515430955
O,0,4.7711300128,-1.1041092524,-0.2166163362
O,0,4.4865749638,1.8658739914,-0.3388576326
C,0,-0.822882931,-0.7445589688,0.3662032095
F,0,-1.4582457858,-1.9157533204,0.157483073
C,0,0.6063077265,-0.8490863436,-0.2455708716
O,0,0.9190200041,-1.7307873133,-0.9925799448
O,0,1.3564053935,0.1569150679,0.1815396486
F,0,-0.7421526735,-0.5363706314,1.7008993977
C,0,-1.6668158078,0.4022788281,-0.2742041081
C,0,-3.2027010087,0.3476933311,0.0070253121
F,0,-1.4950363584,0.3563378326,-1.6153480992
F,0,-1.2103204401,1.586163653,0.178717989
F,0,-3.7694872842,-0.6830716706,-0.6205940548
F,0,-3.7644354277,1.4755559501,-0.4386324899
F,0,-3.4375374024,0.2418164056,1.3177796123
H,0,2.797377371,0.1548334777,-1.3644472474
H,0,3.2720796275,1.5474142403,1.3571904833
H,0,3.5112423761,-0.8844257495,1.4619324422
H,0,5.61227017,-1.0321848362,0.2493047554
H,0,5.3147974943,2.0047813522,0.1350035654

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.9711141
E (total electronic)+ZPVE = -1269.841012
Internal Thermal Energy = -1269.823231
Enthalpy = -1269.822287
Gibbs Free Energy = -1269.890727

C,0,0.1767276602,-2.3076349803,-0.4164644208
C,0,-0.0824595701,-2.7180396344,-1.7397264766
C,0,1.377105329,-3.0432022895,-0.5105552249
O,0,1.6743129679,-3.9505333387,0.4459328625
O,0,-1.268726435,-3.2972664482,-2.0325066851
H,0,-0.5233804528,-2.6651634264,0.3267383586
H,0,0.5422477998,-2.4116795534,-2.56464295
H,0,2.1601538569,-2.7693230698,-1.2010036736
H,0,2.4529239251,-4.4597904844,0.1909114452
H,0,-1.2572178022,-3.6446516335,-2.9325206754
C,0,0.2288870639,1.2901678559,1.3216956186
F,0,0.5744069403,1.607407751,2.5919702031
C,0,0.219436596,-0.271185654,1.1559722012
O,0,0.2551963616,-0.9717694645,2.1459568544
O,0,0.1706852086,-0.611169606,-0.0859844309
F,0,1.1513391333,1.8451426134,0.4943202691
C,0,-1.1581574895,1.9331004642,1.0189036051
C,0,-1.3476164005,3.4056234727,1.5037283235
F,0,-2.1170121038,1.1863398991,1.6174106301
F,0,-1.3731467164,1.9176369095,-0.3125259425
F,0,-0.3504447839,4.1798566107,1.0646162511
F,0,-1.395102482,3.4748319667,2.8350690517
F,0,-2.5000376062,3.8806510402,1.0173058057

B3LYP/6-311+G(3df,2p)
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -457.0607277
E (total electronic) + ZPVE = -456.956686
Internal Thermal Energy = -456.948268
Enthalpy = -456.947324
Gibbs Free Energy = -456.990317

C,0,-0.8166741475,-0.1959761831,-0.2962856437
C,0,-2.0184207812,-0.8202935456,0.3158459149
C,0,1.5267462389,-0.0005062662,-0.2195824458
O,0,1.5261360512,1.0530274499,-0.797917862
O,0,0.4439513151,-0.7244052641,0.0878820996
C,0,-1.6181537352,0.6077655488,0.6768789297
O,0,-2.2976673882,1.7042317115,0.148463684
O,0,-3.0819023204,-1.0785345255,-0.5487592796
H,0,-0.8843238172,0.0947401294,-1.3356155132
H,0,-1.8498157435,-1.5590758582,1.0926373281
H,0,-1.2065508811,0.7387484501,1.6723288816
H,0,-3.1273950948,1.8180953105,0.6248938896
H,0,-3.9077259723,-1.0104748421,-0.0572613367
H,0,2.4228667561,-0.5215731154,0.1324617234

TS–diOHCPr-Formate
E (total electronic) = -457.0245235
E (total electronic) + ZPVE = -456.922860
Internal Thermal Energy = -456.914277
Enthalpy = -456.913333
Gibbs Free Energy = -456.957963

C,0,-1.154118351,0.0165451533,0.0031917991
C,0,-2.2492576947,-0.8209454309,0.2827906596
C,0,-1.7958263287,1.1048638676,0.6224069248
O,0,-1.8529022611,2.2916104519,-0.0100341499
O,0,-2.7676956864,-1.5860515738,-0.6961839015
H,0,-0.9166252786,0.1506792861,-1.0434694058
H,0,-2.5982067726,-0.9936078919,1.2899958312
H,0,-2.1091088006,1.0736819049,1.6553606685
H,0,-2.4166415027,2.9060087903,0.474225702
H,0,-3.5821136649,-2.0086696208,-0.3998998656
C,0,1.4463374633,-0.2423493866,-0.1373543784
O,0,1.4653706702,0.3397080931,-1.2125101211
O,0,0.4125305331,-0.5010644051,0.6007255811
H,0,2.3814699247,-0.617989378,0.3161457062

diOHCPr-2-Methylpropanoate
E (total electronic) = -575.0525547
E (total electronic) + ZPVE = -574.864724
Internal Thermal Energy = -574.851897
Enthalpy = -574.850953
Gibbs Free Energy = -574.905359

C,0,-1.1391072645,0.0676977732,-0.3943860899
C,0,-2.2986731842,-0.8503515718,-0.2417468687
C,0,2.5031051026,-0.4591650205,-0.1283745041
C,0,1.1998903309,0.3107758979,-0.1961961612
O,0,1.0769710781,1.5060221667,-0.0810393198
O,0,0.1477522103,-0.5201470866,-0.3799760898
C,0,-1.9464382212,0.1438424599,0.8617066822
O,0,-2.6857937096,1.3125999291,1.0446292777
O,0,-3.3754763514,-0.6278499425,-1.1012149619
C,0,3.6778360832,0.3932490136,-0.6065677668
C,0,2.7107751954,-0.960743368,1.3136020417
H,0,-1.2532154913,0.8906373783,-1.0869699018
H,0,-2.0813242082,-1.889676456,-0.017412265
H,0,2.393797431,-1.329733851,-0.7771833954
H,0,-1.5145409749,-0.2885156511,1.7584662225
H,0,-3.5030940525,1.0974991242,1.5071242913
H,0,-4.1894206678,-0.8856829736,-0.6551985379
H,0,3.8097289843,1.2691543339,0.0282024137
H,0,4.5956808992,-0.1936066977,-0.5727724477
H,0,3.5320289389,0.7360715402,-1.6310302277
H,0,1.8824730174,-1.5865422121,1.6441814444
H,0,3.6249772867,-1.5515996131,1.3661505657
H,0,2.8086425677,-0.1223681734,2.0046765986

TS–diOHCPr-2-Methylpropanoate
E (total electronic) = -575.0130276
E (total electronic) + ZPVE = -574.827176
Internal Thermal Energy = -574.814417
Enthalpy = -574.813472
Gibbs Free Energy = -574.869212

C,0,0.1474707411,-2.0038837762,-0.5479470133
C,0,-0.8893950246,-2.6564638385,-1.2367950207
C,0,1.1461495697,-2.6975041436,-1.2532262403
O,0,2.1733855277,-3.2488895107,-0.5831720591
O,0,-1.9272615791,-3.1669519842,-0.5507647277
H,0,0.1543150367,-2.1243989102,0.5271477504
H,0,-0.9591346636,-2.647673279,-2.3145108792
H,0,1.1994865144,-2.6908515444,-2.3320322571
H,0,2.7127355944,-3.7883259702,-1.1728323173
H,0,-2.4971952447,-3.6842013073,-1.1317487028
C,0,0.3524822891,1.9314332903,0.3331018832
C,0,0.2512009404,0.412186907,0.5065211672
O,0,0.2687495157,-0.1088191626,1.619667539
O,0,0.1793770364,-0.2410281965,-0.6209557039
C,0,-0.5162106448,2.6734720284,1.3505494122
C,0,1.8275669733,2.3500216298,0.4421340268
H,0,0.0040175881,2.1641964557,-0.6742877779
H,0,-0.443571543,3.7503873217,1.1910471523
H,0,-1.5662306955,2.390712611,1.2618539645
H,0,-0.1933563477,2.457174326,2.3688082455
H,0,1.9266472437,3.4237359172,0.2769637396
H,0,2.2216104296,2.1230798026,1.4340075783
H,0,2.4449217427,1.8375793338,-0.2967717597

diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -614.3777733
E (total electronic) + ZPVE = -614.162342

Internal Thermal Energy = -614.148267
Enthalpy = -614.147322
Gibbs Free Energy = -614.203628

C,0,-1.3445690672,-0.0887643914,-0.356076517
C,0,-2.4406086547,-0.8967776857,0.2417109343
C,0,2.3359723461,-0.1207275455,0.0808104032
C,0,0.9587770227,0.4173243172,-0.3070253162
O,0,0.7341404301,1.4976447624,-0.7967034505
O,0,-0.0217341471,-0.4757849918,-0.0420079241
C,0,-2.2106960066,0.5458071488,0.6843313977
O,0,-3.040699682,1.5775628647,0.2451278179
O,0,-3.4918135751,-1.2338324827,-0.6123886135
C,0,2.6111456606,-1.4168283318,-0.7085017561
C,0,3.3998156616,0.9305232218,-0.2547273479
C,0,2.3489747921,-0.4164342152,1.5944658387
H,0,-1.4878822477,0.2554223114,-1.3714967464
H,0,-2.1590890526,-1.6552071371,0.9650586466
H,0,-1.7889564662,0.667413685,1.6767981679
H,0,-3.8612407383,1.5562840761,0.7495618093
H,0,-4.305155818,-1.2900050568,-0.099289317
H,0,3.6050890784,-1.7876278466,-0.4555653602
H,0,1.8856426878,-2.1920696624,-0.4690293057
H,0,2.5827223588,-1.2380271737,-1.7843775912
H,0,3.2279833597,1.8585234363,0.2896532237
H,0,4.3836638224,0.5502341629,0.0211301806
H,0,3.4094803611,1.1609159894,-1.319591813
H,0,3.3387310791,-0.7723426762,1.8826690422
H,0,2.1326262048,0.4818573575,2.174597692
H,0,1.6205589496,-1.1809603355,1.8585825303

TS–diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -614.3379225
E (total electronic) + ZPVE = -614.124658
Internal Thermal Energy = -614.110585
Enthalpy = -614.109641
Gibbs Free Energy = -614.167096

C,0,-1.8747986017,-0.1633358158,-0.5048253281
C,0,-2.894166626,-1.0954200129,-0.2456742011
C,0,-2.5492197247,0.8756353677,0.1595065192
O,0,-2.6464395134,2.0844870097,-0.4191543512
O,0,-3.3438737583,-1.8845576371,-1.2367328994
H,0,-1.6469773167,0.0202707095,-1.5460581533
H,0,-3.2460820267,-1.2998287578,0.7547836378
H,0,-2.8793408609,0.7839443073,1.1838155552
H,0,-3.2274123501,2.6601361938,0.0917020617
H,0,-4.1181193594,-2.3824966515,-0.9495556552
C,0,2.1244690631,-0.69231179,-0.1251345245
C,0,0.7566857529,-0.1803169588,-0.6388150243
O,0,0.6657055155,0.565122563,-1.611823384
O,0,-0.2602907346,-0.620756819,0.0467315781
C,0,3.2649043692,-0.0553452005,-0.9266931699
C,0,2.1655699625,-2.2232822716,-0.2951952686
C,0,2.2751547082,-0.3327695258,1.3642779226
H,0,4.2239890103,-0.422224951,-0.5564692541
H,0,3.1928261697,-0.3002647446,-1.9858136594
H,0,3.2579557299,1.030603399,-0.8337228037
H,0,3.127836012,-2.6083146838,0.0474728322
H,0,1.3786294899,-2.7061390067,0.282257302
H,0,2.0456256799,-2.5074358808,-1.342451735
H,0,3.2414058053,-0.6818020883,1.7332870128
H,0,2.2299985321,0.7474657804,1.51613425
H,0,1.4923410721,-0.7940145343,1.9638557398

diOHCPr-Fluoroacetate
E (total electronic) = -595.6641607
E (total electronic) + ZPVE = -595.539606
Internal Thermal Energy = -595.528958
Enthalpy = -595.528014
Gibbs Free Energy = -595.577162

C,0,0.1816384251,-0.9578224496,-0.1681647549
C,0,0.8782264819,-1.5014281587,1.0270044803
C,0,-0.8420826839,2.4507329425,-1.0513805198
C,0,-0.8556388452,0.9357087972,-1.1080244167
O,0,-1.5647014277,0.2705418776,-1.813270678
O,0,0.0568372217,0.4533659395,-0.2508635957
C,0,-0.6197354514,-1.725064021,0.8328636816
O,0,-1.1193237271,-2.951802074,0.3991899825
O,0,1.8024579314,-2.5174644549,0.7864933675
F,0,-1.7800054365,2.9652418107,-1.9250711113
H,0,0.3695089729,-1.4463447642,-1.114553705
H,0,1.142488557,-0.7960011904,1.808153958
H,0,-1.0786025981,2.7855397529,-0.0412503049
H,0,0.1436106153,2.8227046786,-1.3315611251
H,0,-1.2639103031,-1.1572224489,1.4962510662
H,0,-1.1430819876,-3.5617983878,1.1444817996
H,0,1.8282522552,-3.1034348497,1.5507298761

TS–diOHCPr-Fluoroacetate
E (total electronic) = -595.6295006
E (total electronic) + ZPVE = -595.506925
Internal Thermal Energy = -595.496268
Enthalpy = -595.495324
Gibbs Free Energy = -595.545646

C,0,0.686046107,-1.3503473995,-0.2085042108
C,0,-0.4251661742,-2.0757886917,-0.6766889096
C,0,1.5538403697,-2.2262770251,-0.8875120839
O,0,2.6048207546,-2.7593968475,-0.2354122825
O,0,-1.3828749561,-2.4579718653,0.19003471
C,0,1.1435690137,2.6022243194,-0.128072527
C,0,1.1862912361,1.1523412444,0.3489497839
O,0,1.5903506832,0.8430560309,1.4578709248
O,0,0.742380175,0.3524051435,-0.5750565403
F,0,1.6257229491,3.4714882569,0.8439722302
H,0,0.8082172592,-1.3149502379,0.8658252793
H,0,-0.6255945342,-2.2013082439,-1.7303327093
H,0,1.5085488502,-2.3623283705,-1.9578008003
H,0,3.0374790497,-3.4266383231,-0.7806723805
H,0,-2.0126304564,-3.0471711224,-0.2411072332
H,0,1.7569217128,2.7148665207,-1.0216871926
H,0,0.1162149605,2.8836166111,-0.3584100581

diOHCPr-Bromoacetate

E (total electronic) = -3069.93957
E (tot. electronic) + ZPVE = -3069.817301
Internal Thermal Energy = -3069.806150
Enthalpy = -3069.805206
Gibbs Free Energy = -3069.857317

C,0,-1.9691868854,-0.2124891818,-0.3048122489
C,0,-3.1962803825,-0.7989130913,0.2948066139
C,0,-2.7524593307,0.6153023713,0.661734587
O,0,-3.3875171771,1.7352500937,0.1276178708
O,0,-4.258030988,-1.0236559988,-0.5807908156
H,0,-2.0183535897,0.0814933341,-1.3444011289
H,0,-3.0588710033,-1.5425774485,1.0730746584
H,0,-2.3477231887,0.7302316409,1.6619728954
H,0,-4.2125080006,1.8840024144,0.6024229797
H,0,-5.0863453671,-0.9264282009,-0.098522155
C,0,1.5744923329,-0.8518209461,0.3284623601
C,0,0.3772492034,-0.0605365467,-0.1566051029
O,0,0.3836688869,1.0204397029,-0.6785733478
O,0,-0.7304331812,-0.7844362995,0.0855781489
H,0,1.6413686779,-1.7907505554,-0.2121874792
H,0,1.4771784247,-1.0611691651,1.3889720238
Br,0,3.2644525685,0.0850008768,0.0731621402

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.9053125
E (tot. electronic) + ZPVE = -3069.785186
Internal Thermal Energy = -3069.773941
Enthalpy = -3069.772997
Gibbs Free Energy = -3069.826930

C,0,-0.3628190658,-1.6240219878,-0.4241965923
C,0,-1.3892446969,-2.2938097926,-1.1163516559
C,0,0.6031650564,-2.3804477262,-1.1150189956
O,0,1.5882612899,-2.9878653091,-0.4264889273
O,0,-2.4230829988,-2.8155551513,-0.4282689923
C,0,0.015424012,2.2663758286,0.2274666048
C,0,0.0847069094,0.7665548701,0.5130984387
O,0,0.474796818,0.2878528634,1.5629876967
O,0,-0.3318688244,0.1108432227,-0.5326675035
Br,0,0.5852116598,3.4021868536,1.7258774361
H,0,-0.3626959982,-1.7459725156,0.6508067667
H,0,-1.4669527414,-2.2690805325,-2.1930861795
H,0,0.6848596999,-2.3599126832,-2.1916484096
H,0,2.1018180299,-3.5613625264,-1.0069112108
H,0,-2.9787066954,-3.3500002301,-1.0072544698
H,0,-1.0032918924,2.556054566,-0.0067738913
H,0,0.6595324381,2.5163632503,-0.6090271151

diOHCPr-Dichloroacetate

E (total electronic) = -1415.6356696
E (tot. electronic) + ZPVE = -1415.522046
Internal Thermal Energy = -1415.509967
Enthalpy = -1415.509023
Gibbs Free Energy = -1415.563439

C,0,-1.2780274538,-0.2040254094,-0.3053172741
C,0,-2.5043926877,-0.7899804737,0.2942311606
C,0,2.3294874269,-0.8425345422,0.2353987764
C,0,1.0637125457,-0.1095402224,-0.206135102
O,0,1.112957272,0.9680445514,-0.7367577902
O,0,-0.0402957263,-0.8002525426,0.0600886994
C,0,-2.0378898157,0.6090556098,0.6919602943
O,0,-2.6607172396,1.7511594574,0.1940384071
O,0,-3.575262284,-0.9806742917,-0.576869955
H,0,-1.3303304535,0.1147152052,-1.3371741156
H,0,-2.366634601,-1.553891675,1.0525398106
H,0,-1.6194367118,0.6909796608,1.6898015098
H,0,-3.4745072298,1.9042172844,0.6866454278
H,0,-4.398639842,-0.8957149952,-0.0839846583
Cl,0,2.503363807,-2.3896618242,-0.6409715739
Cl,0,2.3328563594,-1.0810881306,2.0062436229
H,0,3.1875819142,-0.2319561221,-0.0111738498

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.6039742
E (tot. electronic) + ZPVE = -1415.492331
Internal Thermal Energy = -1415.480236
Enthalpy = -1415.479292
Gibbs Free Energy = -1415.534587

C,0,-0.3736496319,-1.316301094,0.389711993
C,0,-1.2598974293,-2.0482748504,-0.4236005625
C,0,0.660584891,-2.1851738793,-0.0118199253
O,0,1.44473147,-2.760569378,0.9212898592
O,0,-2.425412351,-2.4862405676,0.0940191697
C,0,0.3531274929,2.6098864041,0.7096914846
C,0,0.2580442824,1.1038123569,1.0371532684
O,0,0.6747375113,0.7314370833,2.1216590141
O,0,-0.2617088084,0.3882008861,0.1000390525
Cl,0,-1.2684635877,3.3085145781,0.4088633673
Cl,0,1.4448720032,2.884649208,-0.684672496
H,0,-0.5960739956,-1.3236567114,1.4484518482
H,0,-1.1273743916,-2.1226884243,-1.4924075043
H,0,0.9671843067,-2.2689258991,-1.0436204751
H,0,2.0226352745,-3.4175806679,0.5163266247
H,0,-2.8676045636,-3.0779655735,-0.5254583655
H,0,0.7760045272,3.1390015289,1.5530536471

diOHCPr-Trifluoroacetate

E (total electronic) = -794.2219924
E (total electronic) + ZPVE = -794.113595
Internal Thermal Energy = -794.101611
Enthalpy = -794.100667
Gibbs Free Energy = -794.153891

C,0,-0.7790425635,-0.151098267,-0.3884392374
C,0,-1.9692169851,-0.7895775214,0.2290341717
C,0,2.8373838222,-0.6662152786,0.1794816843
C,0,1.5550756183,0.062435912,-0.3083455414
O,0,1.5814217939,1.1234778063,-0.8600500705
O,0,0.494546715,-0.6757678502,-0.0187837691

C,0,-1.5728622204,0.6378245412,0.6016209364
O,0,-2.2537311283,1.7383016722,0.0884878597
O,0,-3.0329891617,-1.0488350529,-0.6315844748
F,0,3.9177445714,0.05948261,-0.0955236502
F,0,2.9663366782,-1.8578030876,-0.4204323134
F,0,2.7932167951,-0.871114683,1.5032529758
H,0,-0.8481768905,0.1462521347,-1.4254057138
H,0,-1.7869299915,-1.5321207696,0.9990832963
H,0,-1.1533133921,0.7560872783,1.5953171324
H,0,-3.0768339368,1.853651705,0.5761459356
H,0,-3.8572437241,-0.9905161493,-0.1361422216

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -794.1931804
E (total electronic) + ZPVE = -794.086801
Internal Thermal Energy = -794.074792
Enthalpy = -794.073848
Gibbs Free Energy = -794.128229

C,0,-1.0561227126,-0.4548999407,-0.283878008
C,0,-2.2259577143,-1.1497438466,0.0822127508
C,0,-1.5770740744,0.6478503147,0.42471267
O,0,-1.6416119862,1.8526564655,-0.178974629
O,0,-2.9513127198,-1.7713709262,-0.8714477062
H,0,-0.9204553556,-0.297885752,-1.3457544496
H,0,-2.4602205754,-1.3701940469,1.1126855031
H,0,-1.7405333271,0.6130297414,1.4912863837
H,0,-2.1268209385,2.4778399394,0.37161289
H,0,-3.7837090237,-2.091214666,-0.5050430804
C,0,2.8022273431,-1.3673511187,0.0996673083
C,0,1.5092311904,-0.6384611222,-0.3894532634
O,0,1.5977640294,0.2907318604,-1.1636409502
O,0,0.4600938245,-1.1669901837,0.1371130393
F,0,2.7813874895,-2.6678966083,-0.2436246025
F,0,3.905175284,-0.8280884021,-0.4264231311
F,0,2.9162812666,-1.3040407083,1.438277275

diOHCPr-Trichloroacetate

E (total electronic) = -1875.2456093
E (tot. electronic) + ZPVE = -1875.142664
Internal Thermal Energy = -1875.129308
Enthalpy = -1875.128364
Gibbs Free Energy = -1875.185296

C,0,-0.9243435722,0.0210878655,-0.592838525
C,0,-2.1167771785,-0.6259639296,0.0111985965
C,0,2.7021495831,-0.4931307106,-0.0186023657
C,0,1.4068553477,0.2324683553,-0.4943496619
O,0,1.408657512,1.3084473813,-1.0167369658
O,0,0.3443174146,-0.5169402883,-0.2329509875
C,0,-1.7174316693,0.7934294636,0.4108306059
O,0,-2.3965648012,1.9045068856,-0.0822709283
O,0,-3.1817622426,-0.866491295,-0.8538267667
Cl,0,4.1236107142,0.4885976872,-0.4049687397
Cl,0,2.8257483601,-2.0736866268,-0.8430391895
Cl,0,2.6026127043,-0.7308640107,1.7513079753
H,0,-0.9933220326,0.3390481325,-1.6238090079
H,0,-1.9369167979,-1.3834172265,0.7671438599
H,0,-1.2990534751,0.8927649417,1.4070704836
H,0,-3.2223434729,2.0087293496,0.4032181972
H,0,-4.0049253939,-0.8219779748,-0.35515358

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1875.216387
E (tot. electronic) + ZPVE = -1875.115366
Internal Thermal Energy = -1875.102042
Enthalpy = -1875.101097
Gibbs Free Energy = -1875.159426

C,0,-1.2304470395,-0.2736335869,-0.4845116407
C,0,-2.4003210738,-0.9841830326,-0.1502872983
C,0,-1.7566603671,0.8083668355,0.2516565337
O,0,-1.8163350656,2.0302284336,-0.3165850422
O,0,-3.1131557543,-1.581246218,-1.1284062215
H,0,-1.0860896894,-0.0842876963,-1.5400155802
H,0,-2.6466304109,-1.2324300046,0.871007975
H,0,-1.9331267214,0.7416742159,1.3146269393
H,0,-2.306819131,2.6389388962,0.2476169868
H,0,-3.9477286978,-1.9147757319,-0.779664877
C,0,2.6456663491,-1.1795807829,-0.1075770603
C,0,1.3288486193,-0.45015011,-0.5863208314
O,0,1.39830008,0.4955832532,-1.3395406051
O,0,0.2812990883,-0.9931538905,-0.0730025995
Cl,0,4.0896933943,-0.4465195787,-0.8403132304
Cl,0,2.5660857803,-2.9057161488,-0.5789488277
Cl,0,2.7648536394,-1.0471198533,1.6753843795

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.9672607
E (tot. electronic) + ZPVE = -1269.834859
Internal Thermal Energy = -1269.817100
Enthalpy = -1269.816156
Gibbs Free Energy = -1269.884029

C,0,2.7033548818,0.20028262,-0.2925883144
C,0,3.6384197139,1.0844282237,0.4492866152
C,0,3.787407997,-0.4344064078,0.5155230588
O,0,4.768743115,-1.1014732193,-0.2120110193
O,0,4.48374269,1.8657398546,-0.3344085745
C,0,-0.8213099073,-0.7483357831,0.3614977796
F,0,-1.4557383696,-1.9159284659,0.1499975954
C,0,0.6089667628,-0.8522043188,-0.2487038175
O,0,0.9246181875,-1.7362965361,-0.989269691
O,0,1.3552955804,0.156377635,0.1732132731
F,0,-0.741438448,-0.5430586736,1.6936930396
C,0,-1.6637378769,0.4012070642,-0.2768111921
C,0,-3.1987387172,0.3512467531,0.0125078566
F,0,-1.4996486343,0.3526096034,-1.6156814868
F,0,-1.2034462263,1.5815252799,0.1720811812
F,0,-3.7700484086,-0.6783309543,-0.6065586245
F,0,-3.7579802033,1.4765338923,-0.4344263856
F,0,-3.4263055425,0.2523859968,1.3221829711
H,0,2.7978463601,0.1549839677,-1.368492193
H,0,3.2637965456,1.5488228922,1.3557039779

H,0,3.5039704809,-0.8851376986,1.460967986
H,0,5.6088024808,-1.0281370342,0.2541876383
H,0,5.3104835381,2.0048913091,0.1405493259

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.938891
E (tot. electronic) + ZPVE = -1269.808492
Internal Thermal Energy = -1269.790744
Enthalpy = -1269.789800
Gibbs Free Energy = -1269.858202

C,0,0.1729065742,-2.3090338566,-0.4155998091
C,0,-0.0832315799,-2.7152556742,-1.7404068376
C,0,1.3758536303,-3.0400145125,-0.5083033349
O,0,1.6750584336,-3.945649954,0.4460735687
O,0,-1.266557808,-3.2932705203,-2.0376349795
H,0,-0.5281429287,-2.6679282906,0.3262839403
H,0,0.543561493,-2.4065539745,-2.5633000335
H,0,2.158929486,-2.7631986575,-1.1980980772
H,0,2.454514891,-4.4531849909,0.1928448892
H,0,-1.2543931812,-3.6383874661,-2.9377773453
C,0,0.2276813457,1.2865768555,1.325031732
F,0,0.5720235511,1.6026117173,2.5925683915
C,0,0.2188665845,-0.2749867493,1.1579733966
O,0,0.2632554118,-0.9754638072,2.1458829079
O,0,0.1618576846,-0.6136617333,-0.0818548796
F,0,1.1480428802,1.8402328328,0.4992643543
C,0,-1.1595346771,1.9294163553,1.0212528242
C,0,-1.3445941209,3.4053744886,1.4986666265
F,0,-2.1160008398,1.1898086269,1.6254288225
F,0,-1.3769262715,1.9083495361,-0.306450756
F,0,-0.3515049934,4.1740875899,1.0493482704
F,0,-1.3844565497,3.4826582973,2.8268104344
F,0,-2.4970880158,3.8768228874,1.0165968942

mPW3PBE/6-311+G(3df,2p) IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.7583317
E (total electronic) + ZPVE = -456.653794
Internal Thermal Energy = -456.645405
Enthalpy = -456.644461
Gibbs Free Energy = -456.687433

C,0,0.4545392934,-0.2326823167,-0.903398958
C,0,0.5326062828,1.2462309434,-0.9821425172
C,0,-0.9151680256,-2.1151347228,-1.0737064322
O,0,-0.1806353218,-2.786108698,-0.4024919513
O,0,-0.7186346433,-0.8379427727,-1.402355468
C,0,0.4108137013,0.5498779348,0.365847508
O,0,1.5071076281,0.4101497784,1.20278717
O,0,1.7415373075,1.770654057,-1.4148567731
H,0,1.3669917418,-0.7845196528,-1.0948679799
H,0,-0.3620558666,1.7678166652,-1.3135764054
H,0,-1.8540960628,-2.4650559481,-1.5196789092
H,0,-0.5563226091,0.6486000085,0.8527426045
H,0,1.6691209931,1.250398044,1.6426947841
H,0,1.8769295812,2.6236016798,-0.9908546722

TS–diOHCPr-Formate
E (total electronic) = -456.7168077
E (total electronic) + ZPVE = -456.614829
Internal Thermal Energy = -456.606228
Enthalpy = -456.605283
Gibbs Free Energy = -456.650231

C,0,-0.6556051497,0.4177419485,0.2002963365
C,0,-1.7727510133,-0.2259158737,-0.3489819421
C,0,0.2318617238,-0.4919686361,-0.3903216717
O,0,1.2158541336,-1.0290808248,0.3371384673
O,0,-2.832435455,-0.4919852924,0.420661101
C,0,-0.2886514047,2.943812233,0.8277381648
O,0,-0.2826099699,2.6543945382,2.0159991727
O,0,-0.4352496334,2.1478334013,-0.1748717537
H,0,-0.6233848152,0.4892123013,1.2813224779
H,0,-1.8686367652,-0.3991021341,-1.4133835974
H,0,0.2361426306,-0.6778880665,-1.4568732696
H,0,1.674521838,-1.7090766952,-0.1674920829
H,0,-3.4720157781,-1.027048371,-0.0611323992
H,0,-0.1573893415,3.9977644714,0.5101909964

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.6656088
E (total electronic) + ZPVE = -574.477170
Internal Thermal Energy = -574.464453
Enthalpy = -574.463508
Gibbs Free Energy = -574.517374

C,0,-1.126450049,0.0545082681,-0.3978106991
C,0,-2.2850851213,-0.8544549475,-0.2170144884
C,0,2.4970618229,-0.4550737606,-0.1435985675
C,0,1.195476785,0.3054359853,-0.2227841971
O,0,1.0672246083,1.5008131967,-0.1357082159
O,0,0.1517250869,-0.5319442995,-0.381561212
C,0,-1.9227582986,0.1585601258,0.8595885816
O,0,-2.6556074348,1.3251211191,1.0225142611
O,0,-3.3634432453,-0.6480106393,-1.0658616959
C,0,3.6698915139,0.4105291297,-0.57785282
C,0,2.6757889277,-0.9784679886,1.287125914
H,0,-1.2492810131,0.8660800419,-1.1053821723
H,0,-2.0632675249,-1.8899078445,0.0300387455
H,0,2.4039671579,-1.3157515362,-0.8114194466
H,0,-1.4812384383,-0.2601284373,1.7608078483
H,0,-3.4753446879,1.1141940672,1.4798692867
H,0,-4.1708480184,-0.8891989319,-0.6018484375
H,0,3.7792096202,1.2762415907,0.0772990293
H,0,4.5930564477,-0.1695237218,-0.5331488277
H,0,3.544891797,0.7726569417,-1.5996147749
H,0,1.8434322736,-1.614722187,1.5904070693
H,0,3.5934987468,-1.5652493783,1.3498871838
H,0,2.7546740436,-0.1501397936,1.9947386356

TS–diOHCPr-2-Methylpropanoate
E (total electronic) = -574.620428
E (total electronic) + ZPVE = -574.434075
Internal Thermal Energy = -574.421396
Enthalpy = -574.420452
Gibbs Free Energy = -574.474786

C,0,-1.5153193112,0.1225529039,0.0144586117
C,0,-2.5039255509,-0.8665760135,0.0799021373
C,0,-2.2302209671,1.0338436471,0.8012146286
O,0,-2.3075324234,2.3147862339,0.4341332328
O,0,-2.8621489854,-1.5268578892,-1.023452336
C,0,2.4839429692,-0.4350745037,0.3776303018
C,0,1.1152076812,-0.0975252737,-0.2131764826
O,0,1.0103003871,0.3872723552,-1.3382476685
O,0,0.1254853371,-0.337614369,0.5883593951
C,0,3.4306651231,-0.9986189248,-0.6729396612
C,0,3.0606654456,0.8238279889,1.0300292138
H,0,-1.2200947609,0.4565908216,-0.9736236119
H,0,-2.9153749179,-1.2041289445,1.022934067
H,0,-2.6316889537,0.7634320182,1.7699949239
H,0,-2.9133663486,2.7949547276,1.0086736891
H,0,-3.618668325,-2.09610614,-0.8457723192
H,0,2.3205840336,-1.1821776756,1.1588516877
H,0,4.3937925265,-1.2446607319,-0.2197898202
H,0,3.0306844157,-1.9071205499,-1.1284296152
H,0,3.6037569998,-0.2716349429,-1.4682791315
H,0,4.0216452017,0.6005672253,1.4987174439
H,0,3.2238045242,1.6050511224,0.2835571006
H,0,2.3939498666,1.2190639304,1.7990894343

diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -613.9632789
E (total electronic) + ZPVE = -613.747397

Internal Thermal Energy = -613.733333
Enthalpy = -613.732389
Gibbs Free Energy = -613.788663

C,0,-1.2992735709,0.2750601063,-0.7046866774
C,0,-2.4931908206,-0.4338715941,-0.1810275453
C,0,2.3171722407,-0.0868579149,-0.1024816168
C,0,1.0164053503,0.5711505359,-0.5401909405
O,0,0.9078677454,1.6734889512,-1.0160287464
O,0,-0.0423037531,-0.2367815479,-0.3397191639
C,0,-2.1523111088,0.9680195082,0.3040254294
O,0,-2.8554472633,2.0748885913,-0.1489109286
O,0,-3.5217289592,-0.6515231842,-1.0872123095
C,0,2.5148549868,-1.3842148641,-0.8986884121
C,0,3.4753983336,0.8699311292,-0.3681346709
C,0,2.2318711811,-0.4041859697,1.3970545975
H,0,-1.3638097855,0.6529060723,-1.7184138785
H,0,-2.3166797648,-1.2279057257,0.5406148654
H,0,-1.7684839671,1.0266022356,1.3197092025
H,0,-3.7005051938,2.1133204615,0.3093210863
H,0,-4.3588580299,-0.6305372569,-0.6137379296
H,0,3.4596340339,-1.8457785245,-0.6038662141
H,0,1.7116546983,-2.0960867577,-0.7084004994
H,0,2.5565088202,-1.1879233087,-1.9724038273
H,0,3.3567851991,1.8020236487,0.1861500907
H,0,4.4104444815,0.4017694431,-0.0545910723
H,0,3.5540055029,1.1146716248,-1.4283730222
H,0,3.1725801189,-0.8529828629,1.7229015555
H,0,2.0693009543,0.5016883731,1.9853647873
H,0,1.4254815699,-1.1055191698,1.6118618403

TS–diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -613.9179133
E (total electronic) + ZPVE = -613.704350
Internal Thermal Energy = -613.690229
Enthalpy = -613.689285
Gibbs Free Energy = -613.747637

C,0,-1.8796064906,-0.0595981814,-0.4753384554
C,0,-2.8532053999,-1.0631387678,-0.5458074726
C,0,-2.6227927811,0.746108544,0.3956519435
O,0,-2.7108472017,2.0601356123,0.1784686821
O,0,-3.1771927981,-1.5984008454,-1.7248744107
H,0,-1.5675885092,0.3899173998,-1.4111616384
H,0,-3.2796775487,-1.5111284405,0.3430217543
H,0,-3.0398078507,0.3603614245,1.3177176937
H,0,-3.3328456246,2.4636204986,0.7935393805
H,0,-3.9275121546,-2.1950919875,-1.6302623737
C,0,2.1230766246,-0.7026394838,-0.1308522462
C,0,0.7568268581,-0.2317439812,-0.6716520819
O,0,0.6655800203,0.4039692141,-1.7198776816
O,0,-0.2457383238,-0.5643017313,0.0776834494
C,0,3.2395243133,-0.3085807979,-1.0926588133
C,0,2.095752345,-2.2260948098,0.0334529477
C,0,2.3593259368,-0.0435484965,1.2332202847
H,0,4.2013794196,-0.6476213316,-0.6992219086
H,0,3.0952654489,-0.7593988477,-2.0760055878
H,0,3.287317269,0.7733171886,-1.2250170409
H,0,3.0580777497,-2.575186166,0.4169450797
H,0,1.3159862042,-2.532948629,0.7309534713
H,0,1.915890128,-2.7243194545,-0.9227622025
H,0,3.3246457463,-0.3604500356,1.6366118207
H,0,2.3731093848,1.0462578986,1.1491997833
H,0,1.5814332346,-0.3224477933,1.9447306229

diOHCPr-Dichloroacetate
E (total electronic) = -1415.1186937
E (tot. electronic) + ZPVE = -1415.004474
Internal Thermal Energy = -1414.992430
Enthalpy = -1414.991486
Gibbs Free Energy = -1415.045612

C,0,-1.2712439043,-0.2106225747,-0.3037568999
C,0,-2.4997169249,-0.7899965419,0.290309474
C,0,2.3165360179,-0.8389887764,0.2361775973
C,0,1.0523027706,-0.1124783268,-0.2063747827
O,0,1.0943966898,0.9643525229,-0.7350082592
O,0,-0.0436192619,-0.8083533272,0.0587464751
C,0,-2.0281980662,0.6013673374,0.691770994
O,0,-2.6428931133,1.7406340699,0.198608685
O,0,-3.564875683,-0.9696931924,-0.57791002
H,0,-1.3255970605,0.1147516552,-1.3355934767
H,0,-2.3628869796,-1.5564615168,1.0493066622
H,0,-1.6080652397,0.6742787274,1.6919816347
H,0,-3.4609832863,1.8848666892,0.6840554251
H,0,-4.3851204943,-0.8705175123,-0.0850411124
Cl,0,2.4847738319,-2.3800835082,-0.6206379212
Cl,0,2.3157452522,-1.0595702257,1.9944026757
H,0,3.1732707315,-0.2246339596,-0.0184737611

TS–diOHCPr-Dichloroacetate
E (total electronic) = -1415.0821691
E (tot. electronic) + ZPVE = -1414.969940
Internal Thermal Energy = -1414.957891
Enthalpy = -1414.956947
Gibbs Free Energy = -1415.012655

C,0,-0.3051123187,-1.3389764419,0.3718609426
C,0,-1.2628683494,-2.0400251912,-0.3760955749
C,0,0.6879860872,-2.2276955964,-0.0686583944
O,0,1.5260060197,-2.7801838119,0.8168060616
O,0,-2.4175871548,-2.4025932024,0.1958668996
C,0,0.3231984461,2.6149393555,0.7177242248
C,0,0.1947264359,1.1155396511,1.0518528343
O,0,0.4129350407,0.7746954432,2.2025042739
O,0,-0.13529209,0.3800329714,0.0551465684
Cl,0,-1.230651483,3.2696433301,0.1586482817
Cl,0,1.6026611404,2.881167398,-0.4856372131
H,0,-0.4641057074,-1.3053921899,1.4435911126
H,0,-1.1705594363,-2.1660837824,-1.4470565635
H,0,0.9052611749,-2.3634891429,-1.1202599626
H,0,2.0741340423,-3.4463340905,0.3886535137
H,0,-2.9204097332,-2.9701669182,-0.3976932303
H,0,0.6014148856,3.1630472184,1.6114262256

diOHCPr-Trifluoroacetate

E (total electronic) = -793.7217587
E (total electronic) + ZPVE = -793.612631
Internal Thermal Energy = -793.600679
Enthalpy = -793.599735
Gibbs Free Energy = -793.652917

C,0,-0.7725359428,-0.1591192044,-0.3849471048
C,0,-1.9663073771,-0.7888786887,0.2272280006
C,0,2.826335357,-0.6610313153,0.1793393021
C,0,1.54284027,0.0583978238,-0.304456569
O,0,1.559906666,1.1194522565,-0.8534746357
O,0,0.4903872051,-0.6848765533,-0.0160279689
C,0,-1.5644902175,0.6323891616,0.5995079197
O,0,-2.2350603464,1.7297020531,0.0865157908
O,0,-3.0233549846,-1.0401264476,-0.6318092913
F,0,3.8957952857,0.0685652141,-0.0997064536
F,0,2.9573566077,-1.8472944598,-0.4169697693
F,0,2.7847825142,-0.8621216425,1.4976609727
H,0,-0.8434854795,0.1416055055,-1.4229814016
H,0,-1.7862663886,-1.5312909906,1.0009856409
H,0,-1.1444415738,0.7446205863,1.5960793111
H,0,-3.0601230223,1.8418147268,0.5688900515
H,0,-3.8459525731,-0.9673430258,-0.1381167952

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.6882496
E (total electronic) + ZPVE = -793.581172
Internal Thermal Energy = -793.569203
Enthalpy = -793.568258
Gibbs Free Energy = -793.623440

C,0,1.1481227584,-0.1112744308,0.0355332507
C,0,2.1918697892,-0.970018761,-0.3437528043
C,0,1.9083019135,0.9669108219,-0.4473048024
O,0,2.089406584,2.0485996843,0.3217802559
O,0,2.6639993743,-1.866726178,0.5328446439
H,0,0.9167477592,-0.0830915139,1.0940140835
H,0,2.5174227202,-1.0521118946,-1.3725477319
H,0,2.2091458324,1.0307226245,-1.4849726156
H,0,2.7162544244,2.6510875496,-0.0922190045
H,0,3.4464507976,-2.3012832687,0.1774862682
C,0,-2.7849860169,-0.2962334388,-0.6367562482
C,0,-1.4305101298,0.0403036976,0.0565110149
O,0,-1.4294879399,0.6780569548,1.088177795
O,0,-0.4457586387,-0.4359868925,-0.6102216949
F,0,-3.8222213199,0.1802568989,0.0465026925
F,0,-2.9489530122,-1.6201806793,-0.7541486309
F,0,-2.8341424361,0.2274049161,-1.8687033319

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.1829508
E (tot. electronic) + ZPVE = -1269.049538
Internal Thermal Energy = -1269.031807
Enthalpy = -1269.030863
Gibbs Free Energy = -1269.099051

C,0,2.684599972,0.2076172218,-0.2830047268
C,0,3.6307248698,1.0747283675,0.4588197397
C,0,3.7708645055,-0.4411714346,0.5048676246
O,0,4.7372524348,-1.0998142029,-0.2358265522
O,0,4.4699745385,1.855321003,-0.3186283333
C,0,-0.8191116769,-0.7425797438,0.365226949
F,0,-1.4446875586,-1.9063750447,0.1484127976
C,0,0.6058089764,-0.8359718106,-0.2447162329
O,0,0.9228692378,-1.706973329,-0.9979470338
O,0,1.3487193047,0.1649109811,0.1892250445
F,0,-0.7410058841,-0.5387283684,1.6907215376
C,0,-1.6569092913,0.4037614561,-0.2734270217
C,0,-3.1890299205,0.3427120265,0.0043193661
F,0,-1.4834205499,0.3618245873,-1.6047619537
F,0,-1.2074652382,1.5773645115,0.1852973606
F,0,-3.7475163831,-0.6767203939,-0.6310575544
F,0,-3.7465218435,1.4673906825,-0.429647952
F,0,-3.4230584143,0.225328799,1.3055339935
H,0,2.7759800898,0.1743259533,-1.3616955297
H,0,3.263634012,1.5272612017,1.3768519767
H,0,3.4894370971,-0.8998066138,1.449625819
H,0,5.5810108192,-1.0245885074,0.2205207182
H,0,5.303103903,1.9718576579,0.1484479633

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.1499545
E (tot. electronic) + ZPVE = -1269.018383
Internal Thermal Energy = -1269.000753
Enthalpy = -1268.999809
Gibbs Free Energy = -1269.067563

C,0,-3.0229875368,0.1442366841,0.0402465348
C,0,-3.6206820605,1.3716717018,-0.2884601607
C,0,-4.0451480564,-0.4940359575,-0.6817101321
O,0,-4.722711075,-1.5043744392,-0.1190030637
O,0,-3.8652854846,2.2686908266,0.6771961538
C,0,0.8419982946,-0.899403777,-0.0757928665
F,0,1.4982062307,-1.8034287063,0.6724881638
C,0,-0.6378989968,-0.7810710558,0.4191508043
O,0,-0.9506341639,-1.3066189238,1.4652996183
O,0,-1.3505803792,-0.1031342468,-0.4013776754
F,0,0.8704117999,-1.3243681458,-1.3551820429
C,0,1.6021939626,0.4532804156,0.0130528344
C,0,3.1545110843,0.3558627943,-0.0740336494
F,0,1.3037618511,1.0355418049,1.1887392052
F,0,1.1962939953,1.2559460081,-0.9788650609
F,0,3.6625584457,-0.1985606747,1.017506919
F,0,3.6585906391,1.5804157148,-0.1946550673
F,0,3.5200583041,-0.3581178727,-1.1328493228
H,0,-2.9752702935,-0.0948134696,1.0965399484
H,0,-3.7321347535,1.6954755579,-1.3151384537
H,0,-4.1890308766,-0.3201904494,-1.7400874512
H,0,-5.4592949525,-1.7657403768,-0.6815771455
H,0,-4.3760329781,3.0053695872,0.3256359102

B97D/AUG-cc-pVTZ
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.7842243
E (total electronic) + ZPVE = -456.683337
Internal Thermal Energy = -456.674694
Enthalpy = -456.673750
Gibbs Free Energy = -456.717346

C,0,-0.8229154898,-0.2179423407,-0.3175386355
C,0,-2.025635705,-0.8303264128,0.3162293608
C,0,1.5284193948,0.0172213061,-0.2051769875
O,0,1.5149816564,1.1084649096,-0.7274548182
O,0,0.4514282412,-0.7577094266,0.0541107079
C,0,-1.6039463161,0.6043303529,0.6637669391
O,0,-2.2802369788,1.7147843811,0.1349166938
O,0,-3.10918172,-1.0894906705,-0.5388690902
H,0,-0.8995196401,0.0719819583,-1.3623998519
H,0,-1.8546775906,-1.5643594829,1.1055601211
H,0,-1.1776202829,0.7332218444,1.6600634124
H,0,-3.1198432129,1.8023602934,0.607125814
H,0,-3.9220853788,-0.9736220007,-0.0277272423
H,0,2.4319035025,-0.5131457115,0.1333639465

TS–diOHCPr-Formate
E (total electronic) = -456.7583717
E (total electronic) + ZPVE = -456.659075
Internal Thermal Energy = -456.650481
Enthalpy = -456.649536
Gibbs Free Energy = -456.693309

C,0,-1.1348667184,-0.0746211869,-0.0366554673
C,0,-2.2789899776,-0.8472519936,0.2959025487
C,0,-1.7353335073,1.0532227222,0.5843987069
O,0,-1.8081198425,2.2264084083,-0.0962492132
O,0,-2.8958932797,-1.5699173747,-0.6762065262
H,0,-0.9644626217,0.044734386,-1.1047183544
H,0,-2.5833535616,-1.0274771375,1.3224682439
H,0,-1.9776111958,1.0726995513,1.6427619809
H,0,-2.3494731118,2.8532443376,0.4042876912
H,0,-3.7261905252,-1.927464803,-0.3306907637
C,0,1.4522100796,-0.1473109073,-0.0931941627
O,0,1.4749740369,0.6982000854,-0.9835080161
O,0,0.4008740894,-0.6652818304,0.4959405084
H,0,2.3894483857,-0.5767643977,0.3208538736

diOHCPr-Acetate
E (total electronic) = -496.0936803
E (total electronic) + ZPVE = -495.966462
Internal Thermal Energy = -495.955877
Enthalpy = -495.954933
Gibbs Free Energy = -496.004003

C,0,-0.8270549252,-0.2235727139,-0.3251525449
C,0,-2.0343871927,-0.8343105716,0.3037961206
C,0,2.7876639147,-0.6747618548,0.2627573006
C,0,1.5275642388,0.0184055237,-0.1913258207
O,0,1.4600434736,1.1212765363,-0.6959185153
O,0,0.4378448159,-0.7733033715,0.0386551612
C,0,-1.6038148512,0.5942779984,0.6632958141
O,0,-2.2773956038,1.7133213545,0.1467666392
O,0,-3.1219544727,-1.0779083263,-0.5523348062
H,0,-0.9082247725,0.0770739933,-1.3670246226
H,0,-1.8689605671,-1.5777585923,1.0855609408
H,0,2.7292230036,-0.8770591476,1.3384975774
H,0,2.8886324402,-1.6387856775,-0.2482405947
H,0,-1.1756027444,0.7127451369,1.6601671367
H,0,-3.1139610463,1.8011179969,0.6239890496
H,0,-3.9330208201,-0.9494892172,-0.0415350918
H,0,3.651917599,-0.044001167,0.048137756

TS–diOHCPr-Acetate
E (total electronic) = -496.0649514
E (total electronic) + ZPVE = -495.938938
Internal Thermal Energy = -495.928580
Enthalpy = -495.927636
Gibbs Free Energy = -495.976695

C,0,-0.5778776074,-1.0460950645,-0.5032998781
C,0,-1.0534240023,-1.6765932982,-1.6820424974
C,0,0.6097810422,-1.8227261871,-0.523097452
O,0,1.0074505079,-2.462360192,0.6048816454
O,0,-2.3175134039,-2.1709524297,-1.7069729345
H,0,-1.1973427376,-1.2003318918,0.377869099
H,0,-0.5073856006,-1.6509586077,-2.6203291178
H,0,1.3030212442,-1.8030364678,-1.3589228289
H,0,1.7551379566,-3.0414963097,0.399119885
H,0,-2.4471362471,-2.6809350763,-2.519326482
C,0,-0.3169464269,2.8152320707,0.4848286426
C,0,-0.4323160452,1.3005373382,0.627851527
O,0,-0.4654956208,0.7425280626,1.7281609428
O,0,-0.4802214715,0.6873244398,-0.5400789828
H,0,0.6344977003,3.0637483103,-0.0009960935
H,0,-1.1210929156,3.1970451942,-0.1544117556
H,0,-0.3613533721,3.293597109,1.4666782805

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.6921363
E (total electronic) + ZPVE = -574.509697
Internal Thermal Energy = -574.496483
Enthalpy = -574.495539
Gibbs Free Energy = -574.550801

C,0,-1.1511777254,0.0054817916,-0.4510484101
C,0,-2.303775471,-0.8861069103,-0.1311950789
C,0,2.5023266688,-0.4795372911,-0.115401928
C,0,1.1970740594,0.282500006,-0.2741612408
O,0,1.0653991074,1.4898403834,-0.243826408
O,0,0.1472856681,-0.5825734401,-0.4132812557
C,0,-1.9013968462,0.2452168905,0.8250964346

O,0,-2.6370490155,1.439753329,0.8968579085
O,0,-3.4257732017,-0.7721146607,-0.9698333846
C,0,3.6933234715,0.3272447846,-0.6457176385
C,0,2.6793615395,-0.8235030592,1.381975063
H,0,-1.294793404,0.7405250237,-1.2394228725
H,0,-2.0740630823,-1.8933594205,0.2208996362
H,0,2.4120631164,-1.4178586066,-0.6738375068
H,0,-1.4246148622,-0.0783389332,1.7521028148
H,0,-3.4482370643,1.2589322486,1.3915471326
H,0,-4.2126848453,-0.939113524,-0.4331109397
H,0,3.7974321494,1.2658213088,-0.0902657811
H,0,4.6119373432,-0.2564507142,-0.5196150995
H,0,3.5720942136,0.5646979026,-1.7086941778
H,0,1.8376500311,-1.4155244913,1.757271541
H,0,3.6012881397,-1.400886627,1.5126279005
H,0,2.7584980098,0.0957620093,1.9746782908

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.6629123
E (total electronic) + ZPVE = -574.481707
Internal Thermal Energy = -574.468784
Enthalpy = -574.467840
Gibbs Free Energy = -574.522639

C,0,-1.4892839319,-0.0567364851,-0.0741941368
C,0,-2.56437886,-0.912039842,0.2786983758
C,0,-2.0878512138,1.0448903154,0.5901149098
O,0,-2.2005180753,2.2322125471,-0.0552476183
O,0,-3.1511929206,-1.6722143415,-0.6801500626
C,0,2.4846859915,-0.4659865207,0.319711889
C,0,1.1194171126,-0.0313502391,-0.2389865475
O,0,1.0224715578,0.7846271375,-1.16021489
O,0,0.1035584152,-0.5846481194,0.395733884
C,0,3.4944765228,-0.7313614035,-0.8053825088
C,0,2.9955969356,0.6346270458,1.2717941791
H,0,-1.3507375536,0.0868782304,-1.1437152835
H,0,-2.8493395847,-1.0993056136,1.3097347585
H,0,-2.3262284618,1.0262846533,1.6496503555
H,0,-2.7346401991,2.8384881566,0.4776765522
H,0,-3.9436825135,-2.0923618533,-0.3164349568
H,0,2.3365936276,-1.3843218453,0.8988484549
H,0,4.4568246283,-1.034613825,-0.3754337458
H,0,3.1462541276,-1.5275218804,-1.4745745802
H,0,3.6475557005,0.1770156994,-1.3988971401
H,0,3.9568545674,0.3336875604,1.7055541463
H,0,3.1428156212,1.5716502286,0.7207865041
H,0,2.2868924735,0.8159474101,2.0887626824

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9922404
E (total electronic) + ZPVE = -613.782645
Internal Thermal Energy = -613.768237
Enthalpy = -613.767293
Gibbs Free Energy = -613.824513

C,0,-1.3575939577,-0.1186011792,-0.3862356401
C,0,-2.4490242132,-0.8974108849,0.2679939895
C,0,2.3322266397,-0.1198639009,0.0744825404
C,0,0.9515366391,0.4146464159,-0.3245461074
O,0,0.7142009576,1.511550591,-0.789977055
O,0,-0.0228171645,-0.5147246977,-0.0896247513
C,0,-2.1879929972,0.5628434866,0.6609057256
O,0,-3.0218645057,1.6003839417,0.2117232594
O,0,-3.5349843651,-1.2523548218,-0.5505893737
C,0,2.638680939,-1.4064975493,-0.7257982453
C,0,3.400976978,0.9417105852,-0.2272374479
C,0,2.3298234546,-0.438533303,1.5876641857
H,0,-1.520758057,0.2021219074,-1.4124439486
H,0,-2.155226389,-1.6371598973,1.0147457373
H,0,-1.7340672507,0.7061623519,1.6431233246
H,0,-3.8487711062,1.5535012375,0.7111731677
H,0,-4.3298687084,-1.2551736206,0.0002305373
H,0,3.6398540651,-1.7595083993,-0.451854255
H,0,1.9136378152,-2.1940858309,-0.4998209551
H,0,2.6244155535,-1.2088103196,-1.8043126334
H,0,3.2113370159,1.8621589988,0.3351969624
H,0,4.3813935411,0.5478132352,0.0636176601
H,0,3.423063791,1.1852894269,-1.2949101973
H,0,3.3283298283,-0.7891880988,1.8740123675
H,0,2.0955421067,0.4571472704,2.1753759138
H,0,1.6008277499,-1.2192931445,1.8248218643

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9626565
E (total electronic) + ZPVE = -613.754562
Internal Thermal Energy = -613.740317
Enthalpy = -613.739373
Gibbs Free Energy = -613.797181

C,0,-1.6904852694,-0.0334755986,-0.0992045032
C,0,-2.6423772334,-1.0453652859,0.1866345074
C,0,-2.3841596123,0.9155635618,0.6950611439
O,0,-2.6516834032,2.1436569527,0.1864289198
O,0,-3.1669519978,-1.771656811,-0.8325339682
H,0,-1.6097368542,0.2358813287,-1.1502812097
H,0,-2.8668536659,-1.3682479165,1.1989202496
H,0,-2.5817990176,0.7572437234,1.7512156901
H,0,-3.2300058777,2.6251100997,0.7952227831
H,0,-3.8879517791,-2.3234619398,-0.4969493832
C,0,2.3345338033,-0.1267618984,0.0597053094
C,0,0.8937124889,0.2861401035,-0.3502954445
O,0,0.6667800809,1.180198425,-1.1702399197
O,0,-0.0348182756,-0.4163559709,0.2692643807
C,0,3.3715817228,0.7331476596,-0.678431335
C,0,2.5542279591,-1.6125411009,-0.2984842982
C,0,2.5023985192,0.0643546385,1.5824393568
H,0,4.3781819676,0.4238308032,-0.3705700198
H,0,3.2842785591,0.6104144413,-1.763576113
H,0,3.2434680288,1.7949276838,-0.440663381
H,0,3.575291662,-1.9039614539,-0.0213147099
H,0,1.8470188684,-2.2524374408,0.238707256
H,0,2.4301789113,-1.7768353653,-1.3763756044
H,0,3.5246940239,-0.2116804903,1.8704450972
H,0,2.3360412839,1.1114999501,1.8654721594
H,0,1.798247147,-0.5655383592,2.1351626565

diOHCPr-Fluoroacetate

E (total electronic) = -595.192790
E (total electronic) + ZPVE = -595.192790
Internal Thermal Energy = -595.181832
Enthalpy = -595.180888
Gibbs Free Energy = -595.230572

C,0,-0.7059048604,-0.8552644434,-0.0503790768
C,0,-0.2852729397,-1.6192394801,-1.259950619
C,0,-0.5855387057,2.7433918618,0.7204692115
C,0,-0.6272396683,1.2488723327,1.0297810228
O,0,-0.6204393608,0.750451196,2.1313850507
O,0,-0.6794996506,0.5726310128,-0.1434397703
C,0,0.5770520957,-1.6277239393,0.010851134
O,0,0.5899980966,-2.7276006033,0.8823336554
O,0,-1.0927280017,-2.7139099763,-1.6082904464
F,0,-0.5340573223,3.4818846338,1.900841307
H,0,-1.5385094982,-1.2499679691,0.5265396431
H,0,0.1290728224,-1.0475187307,-2.0921581218
H,0,0.304164745,2.9709351585,0.1205765773
H,0,-1.4842745473,3.0308488887,0.1612795137
H,0,1.5065374978,-1.0601009829,-0.0586160544
H,0,1.1326514261,-3.4188058752,0.4784812428
H,0,-0.5210411284,-3.3894050839,-1.9984692697

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.2886985
E (total electronic) + ZPVE = -595.169350
Internal Thermal Energy = -595.158545
Enthalpy = -595.157601
Gibbs Free Energy = -595.207829

C,0,-1.1248189616,-0.0792735403,-0.0614338323
C,0,-2.2589022531,-0.8621839742,0.2833098248
C,0,-1.7385367824,1.0314567362,0.5787815549
O,0,-1.8476074165,2.2079581721,-0.0923750173
O,0,-2.8891359102,-1.5785713982,-0.685746646
H,0,-0.9750581304,0.0526438452,-1.1312064469
H,0,-2.5381088242,-1.0607783843,1.3136022384
H,0,-1.9548636576,1.0395588379,1.6428750257
H,0,-2.3937695966,2.8196234777,0.4215274518
H,0,-3.7109934229,-1.9438553381,-0.3285305118
C,0,2.7474708861,-0.6858146541,0.4459185919
C,0,1.4546967203,-0.0875171643,-0.1330619976
O,0,1.4470933912,0.7810466836,-0.9976187643
O,0,0.413412684,-0.6493189135,0.4413544786
F,0,3.8874759542,-0.1082304871,-0.1332635029
H,0,2.784336465,-0.5074106011,1.5272205825
H,0,2.7743468547,-1.7648492975,0.2525249706

diOHCPr-Chloroacetate

E (total electronic) = -955.7296262
E (total electronic) + ZPVE = -955.610433
Internal Thermal Energy = -955.599189
Enthalpy = -955.598244
Gibbs Free Energy = -955.649433

C,0,-0.1713794628,-0.9064579861,0.0301255626
C,0,0.2520977696,-1.6585592753,-1.1858476885
C,0,-0.0449341328,2.677819392,0.820195773
C,0,-0.0851774892,1.1838473129,1.1360921069
O,0,-0.0778970376,0.6620072042,2.225674422
O,0,-0.1398356429,0.5222839986,-0.0480023165
C,0,1.1082828766,-1.6842459333,0.0889909619
O,0,1.1130732182,-2.7937057849,0.9482762354
O,0,-0.5579531577,-2.7460696452,-1.5499935039
Cl,0,0.0443221528,3.7082564262,2.2928963576
H,0,-1.0081030836,-1.3041308762,0.5989921788
H,0,0.6728621586,-1.0794014929,-2.0096369178
H,0,0.8298457194,2.8957828325,0.2030121107
H,0,-0.9454279665,2.9576098581,0.2683123045
H,0,2.0401632239,-1.1193882482,0.0299577124
H,0,1.6542614473,-3.4828087334,0.5388975781
H,0,0.0129574066,-3.4198300488,-1.9443098772

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.7053697
E (total electronic) + ZPVE = -955.587548
Internal Thermal Energy = -955.576415
Enthalpy = -955.575471
Gibbs Free Energy = -955.627019

C,0,-1.5504687925,-0.0864511344,-0.0667410248
C,0,-2.7039020318,-0.8494998898,0.2593822638
C,0,-2.1612206294,1.0316234549,0.564462674
O,0,-2.248424519,2.2088570796,-0.1086971158
O,0,-3.332928342,-1.5510156835,-0.7214609931
H,0,-1.3832001847,0.044648806,-1.1340976053
H,0,-3.0002536047,-1.047800394,1.2849148037
H,0,-2.3907212259,1.0429742586,1.6257509574
H,0,-2.7956279258,2.8262107496,0.3972216845
H,0,-4.1668875205,-1.9014454538,-0.377747526
C,0,2.2831560781,-0.7512821735,0.5346847464
C,0,1.0240781322,-0.1096414488,-0.078914728
O,0,1.0338975975,0.7781054045,-0.9206560064
O,0,-0.0341765888,-0.6800610487,0.4589000632
Cl,0,3.8453029039,-0.0628829597,-0.0849351498
H,0,2.276442374,-0.6089608322,1.6173489133
H,0,2.2943272793,-1.8207947348,0.3141640429

diOHCPr-Bromoacetate

E (total electronic) = -3071.0041494
E (total electronic)+ZPVE = -3070.885154
Internal Thermal Energy = -3070.873806
Enthalpy = -3070.872862
Gibbs Free Energy = -3070.925358

C,0,-0.5393651602,-0.8674815901,-0.5869667282
C,0,-0.1834173809,-1.526845996,-1.8758556967
C,0,-0.3266905036,2.6561792899,0.4921022787
C,0,-0.400860929,1.1500260676,0.6358753776
O,0,-0.3382735975,0.5588623121,1.6928842184
O,0,-0.5474250564,0.5624383,-0.5765929152
C,0,0.764877799,-1.6025791734,-0.6701313384

O,0,0.8672371553,-2.7633046231,0.1116162318
O,0,-0.9825469016,-2.6180745061,-2.2520204694
Br,0,1.5476863398,3.15895011,0.0437074699
H,0,-1.3195175895,-1.3263905663,0.0150832189
H,0,0.1572435464,-0.8819269654,-2.6877246446
H,0,-0.9443237062,3.0317771726,-0.3231900601
H,0,-0.5540930378,3.1398117252,1.4400342549
H,0,1.6714283462,-1.0011039944,-0.7573869817
H,0,1.3927124085,-3.407624972,-0.3825697602
H,0,-0.4214427326,-3.2420365907,-2.7329264556

TS–diOHCPr-Bromoacetate

E (total electronic) = -3070.9787392
E (total electronic)+ZPVE = -3070.861246
Internal Thermal Energy = -3070.849970
Enthalpy = -3070.849026
Gibbs Free Energy = -3070.902368

C,0,-0.6219054291,-1.2246699746,-0.8465980734
C,0,-0.8939997404,-1.8703043132,-2.0816266326
C,0,0.6435470881,-1.8708121745,-0.8125741986
O,0,1.0125365916,-2.5567171813,0.2997190422
O,0,-2.0589271799,-2.5545779398,-2.2302307325
H,0,-1.2867065444,-1.5020854335,-0.0311111723
H,0,-0.2955992199,-1.7001721532,-2.9713644307
H,0,1.4034494807,-1.6951329596,-1.5681197129
H,0,1.8325228596,-3.0383439443,0.1200126039
H,0,-2.035297047,-3.0496044855,-3.0616715453
C,0,-0.5564180898,2.5812745172,0.275481339
C,0,-0.6209585545,1.053423517,0.3607617764
O,0,-0.5679800449,0.4790508413,1.4466323236
O,0,-0.7314201903,0.4926396075,-0.8216143604
Br,0,1.3469166844,3.1363648563,0.0334191824
H,0,-1.0901454186,2.9816191007,-0.5862498472
H,0,-0.8804182453,3.0383051193,1.2099214382

diOHCPr-Dichloroacetate

E (total electronic) = -1415.3633421
E (total electronic)+ZPVE = -1415.253429
Internal Thermal Energy = -1415.240978
Enthalpy = -1415.240034
Gibbs Free Energy = -1415.294860

C,0,-0.4085393988,-0.9120869909,-0.3114388726
C,0,0.143464301,-1.6209563457,-1.500438935
C,0,-0.4505816651,2.6839256857,0.6549613871
C,0,-0.474631229,1.1550730092,0.8151729562
O,0,-0.5354491691,0.6394527845,1.9086800993
O,0,-0.4239984087,0.5206808399,-0.3651504175
C,0,0.8938391558,-1.6379965042,-0.159876109
O,0,0.8730730604,-2.7607366216,0.6800298975
O,0,-0.58908728,-2.7303998623,-1.9484333739
Cl,0,-1.8992931748,3.2582024554,-0.2569223402
Cl,0,1.0939411586,3.2212768921,-0.1112686507
H,0,-1.2737806545,-1.346754454,0.1822584785
H,0,0.6061033032,-1.007122813,-2.2751848314
H,0,-0.4929706774,3.1421682875,1.6399993451
H,0,1.8024682562,-1.0340501687,-0.1337033667
H,0,1.4666169479,-3.42418777,0.3018586037
H,0,0.0382404743,-3.3715074236,-2.3102878704

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3412099
E (total electronic)+ZPVE = -1415.232643
Internal Thermal Energy = -1415.220338
Enthalpy = -1415.219394
Gibbs Free Energy = -1415.274918

C,0,-1.8274444557,0.2211734362,0.0868965844
C,0,-2.6811075791,0.9971623959,-0.7435528648
C,0,-2.5462902828,-0.9150840899,-0.3790279156
O,0,-3.0826846024,-1.778570432,0.5251918514
O,0,-3.3522219082,2.0502992005,-0.2011709977
C,0,2.1186371958,-0.1955240392,0.4184845425
C,0,0.5964726205,-0.2666161602,0.7214814684
O,0,0.2393191369,-0.9075701986,1.7032560781
O,0,-0.1442942866,0.3725085351,-0.1387964274
Cl,0,2.7138779018,1.5133460351,0.3608603175
Cl,0,2.4946430383,-1.08465989,-1.1159087357
H,0,-1.9366680045,0.4109742911,1.1529091142
H,0,-2.6656343961,0.9176861214,-1.8262348603
H,0,-2.5094618278,-1.2355508413,-1.4156460359
H,0,-3.640633418,-2.4182661937,0.060402823
H,0,-3.9904103857,2.3860493468,-0.8464242906
H,0,2.6751212533,-0.6926715173,1.2097963486

diOHCPr-Trifluoroacetate

E (total electronic) = -793.782959
E (total electronic) + ZPVE = -793.678222
Internal Thermal Energy = -793.665899
Enthalpy = -793.664955
Gibbs Free Energy = -793.718934

C,0,-0.7907610416,-0.1747089622,-0.4123286069
C,0,-1.9803562422,-0.7960584492,0.2336382192
C,0,2.847254114,-0.663044648,0.1845821284
C,0,1.5494768081,0.0724570201,-0.2997777705
O,0,1.5595029159,1.1657441652,-0.8055371157
O,0,0.494981442,-0.7119876812,-0.0543380488
C,0,-1.558913315,0.6398419172,0.583905792
O,0,-2.2358377698,1.7529743756,0.0672023303
O,0,-3.0670553745,-1.0601392387,-0.6120741324
F,0,3.9327764794,0.0921858961,-0.0518000361
F,0,3.004595705,-1.8437186148,-0.4594615925
F,0,2.7880341399,-0.9147526581,1.5140757219
H,0,-0.8699319206,0.1164068343,-1.4561614049
H,0,-1.7934514339,-1.5293693871,1.0198956751
H,0,-1.1209183302,0.7595407985,1.5762582438
H,0,-3.0675280999,1.84569723,0.5524604772
H,0,-3.8764820765,-0.9566035978,-0.0928228802

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.7630198

E (total electronic) + ZPVE = -793.659655
Internal Thermal Energy = -793.647472
Enthalpy = -793.646528
Gibbs Free Energy = -793.700886

C,0,-1.038624788,-0.5038254992,-0.3164083759
C,0,-2.2367150716,-1.1528163362,0.091736578
C,0,-1.5461930184,0.6160087845,0.4023475295
O,0,-1.645277424,1.8181553517,-0.2297581388
O,0,-3.0304780903,-1.7289462478,-0.8545187715
H,0,-0.9513895902,-0.3437321243,-1.3892600616
H,0,-2.4319516206,-1.4047003023,1.129585511
H,0,-1.6413342328,0.6100931873,1.4838637907
H,0,-2.1197357545,2.4379648904,0.3420799659
H,0,-3.8627314216,-2.0042967555,-0.4447754535
C,0,2.8115582259,-1.349377053,0.1141327755
C,0,1.5037683587,-0.6194533681,-0.385607147
O,0,1.5803009572,0.3750812153,-1.0855468873
O,0,0.4495785543,-1.2351520769,0.0679510267
F,0,2.8346422009,-2.647497035,-0.2859829662
F,0,3.9264209836,-0.7572875129,-0.3615733392
F,0,2.8865037315,-1.336248118,1.4710619637

diOHCPr-Trichloroacetate

E (total electronic) = -1874.9889202
E (total electronic)+ZPVE = -1874.889498
Internal Thermal Energy = -1874.875774
Enthalpy = -1874.874830
Gibbs Free Energy = -1874.932741

C,0,-0.9409078745,-0.0042432796,-0.6362931643
C,0,-2.1263850378,-0.6344542934,0.0086830527
C,0,2.7057584207,-0.4863038376,-0.0116500219
C,0,1.3942789069,0.2405752312,-0.4966723714
O,0,1.3810763407,1.3561963147,-0.9495712795
O,0,0.3413386858,-0.5624653576,-0.3068990611
C,0,-1.6907476421,0.789184529,0.3904532558
O,0,-2.3689531142,1.9187280259,-0.0879904007
O,0,-3.2272288007,-0.8684805212,-0.8277202423
Cl,0,4.1403362305,0.5159137394,-0.3717932218
Cl,0,2.8707656238,-2.0810833252,-0.8417423819
Cl,0,2.5752700839,-0.7265407448,1.7787008477
H,0,-1.030550133,0.3146890726,-1.6712200957
H,0,-1.9340214212,-1.3895770651,0.772677044
H,0,-1.2385568042,0.8811889624,1.3794601536
H,0,-3.2031467119,1.9912855468,0.3963690344
H,0,-4.0278157525,-0.7780049975,-0.2925681474

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1874.9691493
E (total electronic)+ZPVE = -1874.871139
Internal Thermal Energy = -1874.857520
Enthalpy = -1874.856575
Gibbs Free Energy = -1874.915445

C,0,2.2312989816,0.062110053,-0.2099334775
C,0,3.2541337744,0.9084013567,0.301360507
C,0,2.8736364352,-0.9606344674,0.5458094069
O,0,3.2474148138,-2.1111361161,-0.0793527381
O,0,4.0079444114,1.6340591774,-0.5716836262
H,0,2.2638492127,-0.0909955272,-1.2868968518
H,0,3.3122652426,1.1725482663,1.3527220159
H,0,2.8743304645,-0.9580956284,1.6314746469
H,0,3.7779589224,-2.6437512793,0.5298585168
H,0,4.7393750705,2.0468290835,-0.0911156053
C,0,-1.7378286165,0.1019154744,0.0176092201
C,0,-0.2651133915,-0.3109246588,-0.4439554254
O,0,-0.0897595271,-1.2932104374,-1.1394578124
O,0,0.6168043121,0.5050756699,0.0544545323
Cl,0,-2.0436846577,1.8548885541,-0.3079190039
Cl,0,-2.9868844633,-0.867122424,-0.8361684473
Cl,0,-1.860257955,-0.2189903568,1.8014460321

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.296421
E (tot. electronic) + ZPVE = -1269.168248
Internal Thermal Energy = -1269.150332
Enthalpy = -1269.149388
Gibbs Free Energy = -1269.215740

C,0,2.4500469969,-0.5262188431,0.1099089027
C,0,3.3033672876,-0.0072531683,-0.9946873576
C,0,2.855991383,0.9154532649,0.1509607264
O,0,3.7226717016,1.27300522,1.192313325
O,0,4.6028776824,-0.5287228225,-1.0600559992
C,0,-1.2052788447,-1.2439656602,0.2294273521
F,0,-1.1463171506,-2.3531727173,-0.5660950369
C,0,0.2247562746,-0.9082061413,0.7828267426
O,0,0.4404771177,-0.7168414398,1.9524107331
O,0,1.0956426775,-0.8757374411,-0.2291183243
F,0,-2.0220394959,-1.5200057027,1.2759659569
C,0,-1.8809373663,-0.1020513794,-0.6316500599
C,0,-1.9951921349,1.2984525056,0.0776888934
F,0,-3.1355605016,-0.5061971213,-0.9611540871
F,0,-1.1681559047,0.0708555473,-1.7731855145
F,0,-2.7187203043,1.2105098725,1.2051742084
F,0,-2.5866374488,2.1755814029,-0.7505267753
F,0,-0.7640541045,1.7589765688,0.3851251317
H,0,2.9048956609,-1.1906767325,0.8392687818
H,0,2.8143571805,0.1880283069,-1.9505723643
H,0,2.1043767279,1.6558075332,-0.1262352255
H,0,4.3174951342,1.9594842153,0.8596506167
H,0,5.1806984315,0.1629577322,-1.411120626

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.2768395
E (tot. electronic) + ZPVE = -1269.150285
Internal Thermal Energy = -1269.132410
Enthalpy = -1269.131466
Gibbs Free Energy = -1269.198579

C,0,0.9470590009,2.1503732951,-0.4907186078
F,0,-0.248926839,2.7799327299,-0.2621012298

C,0,0.8117747013,0.6018292671,-0.2032704439
O,0,1.6363155532,0.0404163323,0.4962470898
O,0,-0.223700122,0.109303639,-0.817750165
F,0,1.8632703602,2.696372144,0.3551610482
C,0,1.3743552214,2.5207011045,-1.9640192574
C,0,2.6923235978,1.8310768429,-2.4778761795
F,0,1.5593731778,3.8684365049,-2.0363419447
F,0,0.3760164991,2.1809646643,-2.819686086
F,0,3.7350748765,2.1294703034,-1.6844152489
F,0,2.9655855847,2.2544943356,-3.7258430163
F,0,2.5365023828,0.4918160867,-2.5057900901
C,0,-0.3365718128,-1.5874649888,-0.7811075787
C,0,-1.3896020042,-2.210768191,-1.5063687025
C,0,0.5183153164,-2.4191248344,-1.560028101
O,0,1.4195770308,-3.2196904076,-0.9268636056
O,0,-2.405829206,-2.8023907683,-0.8174401426
H,0,-0.3253976826,-1.8051734281,0.2848503841
H,0,-1.5374297868,-2.0407378681,-2.568349356
H,0,0.6420244334,-2.2736756511,-2.6287709655
H,0,1.8368923116,-3.8023304668,-1.5769562057
H,0,-2.9638965946,-3.2941096455,-1.4365095953

B97D/6-311+G(3df,2p)
IEFPCM, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.7728572
E (total electronic) + ZPVE = -456.671836
Internal Thermal Energy = -456.663205
Enthalpy = -456.662261
Gibbs Free Energy = -456.705825

C,0,-0.8230334305,-0.2177289726,-0.3203133559
C,0,-2.0249503883,-0.8299633151,0.3159492296
C,0,1.5254927715,0.0171637061,-0.2033771448
O,0,1.5124221228,1.1089373203,-0.7208847953
O,0,0.4492444329,-0.7572112425,0.0502208604
C,0,-1.6023454664,0.6049135806,0.6627697817
O,0,-2.2792399782,1.7128111266,0.1353876549
O,0,-3.1087601618,-1.0876069193,-0.5355268452
H,0,-0.8990219135,0.071947999,-1.3656432001
H,0,-1.8529887635,-1.5654517292,1.1043626155
H,0,-1.1738659117,0.7355437741,1.6584084334
H,0,-3.1200343493,1.7986613935,0.6043182069
H,0,-3.9209336628,-0.9721734515,-0.0244795776
H,0,2.4290851785,-0.5140742698,0.1347785065

TS–diOHCPr-Formate
E (total electronic) = -456.7464294
E (total electronic) + ZPVE = -456.647017
Internal Thermal Energy = -456.638431
Enthalpy = -456.637487
Gibbs Free Energy = -456.681232

C,0,-1.1364405424,-0.0738407616,-0.0393840924
C,0,-2.2792677689,-0.8475107772,0.294973647
C,0,-1.7348366963,1.0542874693,0.5830968489
O,0,-1.8045691102,2.227091105,-0.0939597806
O,0,-2.8939343167,-1.5726829326,-0.6735517583
H,0,-0.9649943951,0.044635847,-1.1075469475
H,0,-2.5831218556,-1.0264250016,1.3222583525
H,0,-1.9774686277,1.072697303,1.6417545053
H,0,-2.3453238796,2.8544383065,0.4052038758
H,0,-3.7234413115,-1.9311605294,-0.3291146283
C,0,1.4491217092,-0.1467389882,-0.0925561511
O,0,1.4731467688,0.6998461282,-0.9795717528
O,0,0.397948763,-0.6648770091,0.4920602854
H,0,2.386393513,-0.5773402998,0.3217286461

diOHCPr-Acetate
E (total electronic) = -496.0810825
E (total electronic) + ZPVE = -495.953742
Internal Thermal Energy = -495.943192
Enthalpy = -495.942248
Gibbs Free Energy = -495.991130

C,0,-0.8268080143,-0.2232993089,-0.3287672959
C,0,-2.0326361406,-0.8344192265,0.3038038759
C,0,2.7852314792,-0.6749117872,0.2636663322
C,0,1.5251183108,0.019259109,-0.1909347754
O,0,1.458221266,1.1225238301,-0.6907915204
O,0,0.4366237398,-0.7721621222,0.0333335866
C,0,-1.6014000742,0.5943886946,0.6622985286
O,0,-2.2772380179,1.7103394493,0.1482112879
O,0,-3.1213478556,-1.0761999503,-0.5476387341
H,0,-0.9081246542,0.0769112436,-1.3710951784
H,0,-1.8653013668,-1.5795305468,1.0842504986
H,0,2.7266257239,-0.8770260091,1.3394680054
H,0,2.8866457041,-1.6391723674,-0.2467858141
H,0,-1.1700072537,0.7148067629,1.6580616005
H,0,-3.1161267496,1.7933683694,0.6207608633
H,0,-3.931237774,-0.9426597288,-0.0376309952
H,0,3.6502741668,-0.0449485113,0.0498812344

TS–diOHCPr-Acetate
E (total electronic) = -496.0518083
E (total electronic) + ZPVE = -495.925713
Internal Thermal Energy = -495.915372
Enthalpy = -495.914427
Gibbs Free Energy = -495.963341

C,0,-0.5808244482,-1.0478085874,-0.5010278671
C,0,-1.0554228503,-1.6765405532,-1.6812230164
C,0,0.6093360277,-1.8207979222,-0.5218731419
O,0,1.0109354844,-2.4566787112,0.60416879
O,0,-2.3179151383,-2.1688941239,-1.7087852256
H,0,-1.2001764391,-1.202660681,0.3803255356
H,0,-0.5085049379,-1.6491076304,-2.6193252261
H,0,1.3017005218,-1.7991738102,-1.3588219657
H,0,1.7589808273,-3.0344337613,0.3992146476
H,0,-2.44824167,-2.6781617089,-2.5206278296
C,0,-0.3157655393,2.8119560193,0.4833654911
C,0,-0.4330917597,1.2968264001,0.6280834676
O,0,-0.4617903852,0.7405402533,1.7274131251
O,0,-0.4868055482,0.6834223824,-0.5371387531
H,0,0.6401543443,3.0588941841,0.0053708316
H,0,-1.1137881546,3.1945593548,-0.1630483667
H,0,-0.3669973345,3.2925858956,1.4638415031

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.6769702
E (total electronic) + ZPVE = -574.494554
Internal Thermal Energy = -574.481333
Enthalpy = -574.480389
Gibbs Free Energy = -574.535775

C,0,-1.1508059057,0.0068238864,-0.4552206861
C,0,-2.3014350032,-0.8862285112,-0.130276104
C,0,2.5001115402,-0.480703737,-0.1165552318
C,0,1.1948319701,0.2825160418,-0.2743003117
O,0,1.0636993975,1.488122281,-0.238686662
O,0,0.1461805676,-0.5797494546,-0.4189566318
C,0,-1.8974265666,0.2470025684,0.8235454672

O,0,-2.6341927537,1.4381531694,0.8956125386
O,0,-3.4250000483,-0.7742132763,-0.9632371343
C,0,3.6917863206,0.3281968063,-0.6442988056
C,0,2.6763156748,-0.8250917526,1.3816912688
H,0,-1.2951783619,0.7408349409,-1.2448832038
H,0,-2.0693646008,-1.8937433188,0.2210100917
H,0,2.410142327,-1.4189326108,-0.6762425154
H,0,-1.416700066,-0.0733736302,1.7501664756
H,0,-3.4466900808,1.256805359,1.386572386
H,0,-4.2103430352,-0.9388493449,-0.4247429335
H,0,3.7939901282,1.2667121105,-0.0883141956
H,0,4.611205568,-0.2542023698,-0.5170562655
H,0,3.5730489529,0.5663182801,-1.7075570728
H,0,1.834091243,-1.4164019832,1.757421609
H,0,3.5976052746,-1.4035515048,1.5131449858
H,0,2.7562954575,0.0939640505,1.9748079312

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.6472156
E (total electronic) + ZPVE = -574.466024
Internal Thermal Energy = -574.453111
Enthalpy = -574.452167
Gibbs Free Energy = -574.506932

C,0,-1.4893188527,-0.0566196376,-0.0782673644
C,0,-2.5633452805,-0.9138356209,0.2738983305
C,0,-2.0864728256,1.0432579989,0.5905788934
O,0,-2.1964352395,2.2320686332,-0.0478962675
O,0,-3.1477582368,-1.6736774795,-0.6836903606
C,0,2.4816019649,-0.4646196528,0.3234987176
C,0,1.1168970731,-0.0273422437,-0.2360878075
O,0,1.0220520566,0.7936116026,-1.1506567212
O,0,0.1008897417,-0.5856683324,0.3898341033
C,0,3.4887571221,-0.7360406301,-0.8036939781
C,0,2.9981615497,0.6395077428,1.269610436
H,0,-1.3499208879,0.0894356634,-1.1475281363
H,0,-2.8474569209,-1.1031246956,1.3051428842
H,0,-2.3244390367,1.0206140839,1.650474808
H,0,-2.7301319636,2.8371369726,0.4855287859
H,0,-3.939670062,-2.0952633396,-0.3222779943
H,0,2.3316390432,-1.3808659863,0.9065660907
H,0,4.4523960012,-1.0383379729,-0.3756017862
H,0,3.1386969306,-1.5350599684,-1.4688040904
H,0,3.6410058976,0.1695274838,-1.4017859009
H,0,3.9586920924,0.3372732554,1.7044461047
H,0,3.1488322386,1.5731691537,0.7137303382
H,0,2.2914715619,0.8286999852,2.0868161362

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9760274
E (total electronic) + ZPVE = -613.766416
Internal Thermal Energy = -613.752034
Enthalpy = -613.751090
Gibbs Free Energy = -613.808132

C,0,-1.357058047,-0.1236102335,-0.3890223486
C,0,-2.4463882996,-0.8946343981,0.2788800084
C,0,2.3301854897,-0.120820061,0.0744067127
C,0,0.9489886145,0.4119582846,-0.3263370239
O,0,0.7117279787,1.5062014068,-0.7940840394
O,0,-0.0235419406,-0.5160021599,-0.0910238979
C,0,-2.1837397663,0.5704652447,0.6534688279
O,0,-3.0186821402,1.6002305891,0.1954926136
O,0,-3.5342509433,-1.2577942557,-0.5296205806
C,0,2.6414849036,-1.4024288626,-0.7334630509
C,0,3.3973569949,0.9456643847,-0.2187880328
C,0,2.3249618443,-0.4487231661,1.586203977
H,0,-1.5213705408,0.1849710539,-1.4191389481
H,0,-2.1497452603,-1.6268898557,1.0325699602
H,0,-1.7258252486,0.7271772357,1.6322946359
H,0,-3.8462476297,1.5565753683,0.692790322
H,0,-4.327349196,-1.2539431508,0.0225455846
H,0,3.6419974457,-1.7565991111,-0.4581266066
H,0,1.9164205433,-2.1925862972,-0.5160033685
H,0,2.6315279601,-1.197925166,-1.8109202541
H,0,3.2042001031,1.8627451841,0.3481970678
H,0,4.3783548769,0.5530789161,0.0722849598
H,0,3.421807248,1.1956881986,-1.2850137689
H,0,3.3233105954,-0.799700611,1.8731634253
H,0,2.0881009539,0.4429636484,2.17922524
H,0,1.5966518205,-1.2319383855,1.8177352106

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -613.9459075
E (total electronic) + ZPVE = -613.737818
Internal Thermal Energy = -613.723590
Enthalpy = -613.722646
Gibbs Free Energy = -613.780306

C,0,-1.6902037396,-0.0342616548,-0.1032795452
C,0,-2.6411127435,-1.0461043079,0.1868158499
C,0,-2.3790571095,0.9162679636,0.693699715
O,0,-2.6431912248,2.1441638145,0.1886815442
O,0,-3.1658627889,-1.7748432285,-0.8276952806
H,0,-1.6108013995,0.2340085714,-1.1549249131
H,0,-2.8629745163,-1.3672530605,1.2005837245
H,0,-2.5739893257,0.7575478609,1.7506478292
H,0,-3.2188487227,2.6272113982,0.79759735
H,0,-3.8858541332,-2.326220045,-0.4912885577
C,0,2.3319604916,-0.1266655183,0.0589446322
C,0,0.8912515925,0.2857482985,-0.35289899
O,0,0.6656236236,1.1814847606,-1.1689027725
O,0,-0.0365237133,-0.418620102,0.2610788831
C,0,3.3699672774,0.7348045058,-0.6774156574
C,0,2.5534855461,-1.6128015561,-0.2994056191
C,0,2.4965901183,0.0643414442,1.5827624058
H,0,4.3765847132,0.4264304257,-0.3682115151
H,0,3.2849388619,0.6127688598,-1.7629403215
H,0,3.2409191215,1.7965968756,-0.439765289
H,0,3.5740150102,-1.9043612568,-0.0199038009
H,0,1.8453545496,-2.2538632646,0.2353921617
H,0,2.4323946258,-1.7771617171,-1.3777942035
H,0,3.5181940458,-0.2117887129,1.8736438265
H,0,2.3298150796,1.1115435751,1.8660118048
H,0,1.7911367999,-0.5653241896,2.1343263588

diOHCPr-Fluoroacetate

E (total electronic) = -595.2974721
E (total electronic) + ZPVE = -595.176726
Internal Thermal Energy = -595.165763
Enthalpy = -595.164819
Gibbs Free Energy = -595.214500

C,0,-0.7092171257,-0.8557675393,-0.0487518097
C,0,-0.285233394,-1.6173473296,-1.2592305035
C,0,-0.5844305724,2.7411190823,0.7195523134
C,0,-0.6267576002,1.2462653189,1.0299907435
O,0,-0.6163275586,0.749073572,2.1303232031
O,0,-0.6837883835,0.5700651155,-0.1405944085
C,0,0.5758340366,-1.625679356,0.0126922143
O,0,0.5896871722,-2.7257615263,0.880216925
O,0,-1.088000893,-2.7122249007,-1.6085763643
F,0,-0.5296566263,3.4796096777,1.8960465107
H,0,-1.5425753027,-1.2506793017,0.5275390551
H,0,0.127549835,-1.0435365447,-2.0914096962
H,0,0.3041443461,2.9669382294,0.1170600169
H,0,-1.4840737659,3.0287314448,0.1616136283
H,0,1.5048587376,-1.0560150852,-0.0533506897
H,0,1.1287191776,-3.4177697234,0.4745968232
H,0,-0.5157610829,-3.3875431336,-1.9964829617

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.2721678
E (total electronic) + ZPVE = -595.152688
Internal Thermal Energy = -595.141900
Enthalpy = -595.140956
Gibbs Free Energy = -595.191083

C,0,-1.1258604315,-0.0786110397,-0.0645790295
C,0,-2.2581922164,-0.8629159583,0.282450072
C,0,-1.7368558505,1.0322296113,0.5779193621
O,0,-1.8433100848,2.2085504149,-0.0893116549
O,0,-2.8867811297,-1.5814151106,-0.682955257
H,0,-0.9758613239,0.0528811696,-1.1345290264
H,0,-2.5362131931,-1.0604872634,1.3136065888
H,0,-1.9527986035,1.0389047799,1.6424495436
H,0,-2.3881718629,2.8208037564,0.4239126607
H,0,-3.7077439419,-1.9475928765,-0.3265211065
C,0,2.7448289741,-0.6846411337,0.4462649218
C,0,1.4521021252,-0.0867147001,-0.1350048414
O,0,1.4454448036,0.7814950594,-0.9975300569
O,0,0.4117115145,-0.6488771843,0.4356406802
F,0,3.8836478853,-0.1091104341,-0.1294725793
H,0,2.7794673685,-0.5060036371,1.5277793994
H,0,2.7716239671,-1.7640114539,0.2537583233

diOHCPr-Chloroacetate

E (total electronic) = -955.7119919
E (total electronic) + ZPVE = -955.592702
Internal Thermal Energy = -955.581473
Enthalpy = -955.580529
Gibbs Free Energy = -955.631629

C,0,-0.1747855189,-0.9067582063,0.0316258138
C,0,0.2519120885,-1.656692478,-1.1851114937
C,0,-0.0436307213,2.6764507789,0.8209825664
C,0,-0.0847645283,1.1813774377,1.1357607763
O,0,-0.0738095203,0.6607680937,2.2241794059
O,0,-0.1443272128,0.5199282192,-0.0455198737
C,0,1.1069981092,-1.6819238339,0.0908022091
O,0,1.1129207371,-2.7912405316,0.9465359938
O,0,-0.5536088165,-2.7443910547,-1.549975365
Cl,0,0.0479171392,3.7024323138,2.2870483955
H,0,-1.0122294984,-1.3045550634,0.5999667532
H,0,0.6710863764,-1.0756357285,-2.0090154474
H,0,0.8300764788,2.8916571799,0.2004037547
H,0,-0.9440601785,2.9552307894,0.2675041504
H,0,2.0383582655,-1.1150011378,0.0349223532
H,0,1.6514906435,-3.4807782325,0.5361168042
H,0,0.0176141566,-3.4178595458,-1.9425937966

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.6871439
E (total electronic) + ZPVE = -955.569221
Internal Thermal Energy = -955.558108
Enthalpy = -955.557164
Gibbs Free Energy = -955.608609

C,0,-1.5515743567,-0.0860646208,-0.0702476125
C,0,-2.7033555818,-0.8503889671,0.2582291002
C,0,-2.1590722793,1.03233039,0.5633495233
O,0,-2.2432612864,2.2094677751,-0.1056594913
O,0,-3.3309169201,-1.5541747332,-0.7187880944
H,0,-1.3838464274,0.0445026462,-1.1377554588
H,0,-2.9986930043,-1.0473199965,1.2846625213
H,0,-2.3883545383,1.0421655687,1.6250567087
H,0,-2.7887123483,2.8275980176,0.3998273257
H,0,-4.1637917871,-1.9057350889,-0.3755954587
C,0,2.2824143959,-0.7491987666,0.5344176754
C,0,1.02142687,-0.1089448244,-0.0798212399
O,0,1.0323237314,0.7797935288,-0.9182298124
O,0,-0.0357202689,-0.6806542944,0.4527975073
Cl,0,3.8368035065,-0.0639480065,-0.0829896077
H,0,2.2725414787,-0.6070179855,1.6176175268
H,0,2.291181816,-1.8198266428,0.3167088871

diOHCPr-Bromoacetate

E (total electronic) = -3070.9193034
E (total electronic)+ZPVE = -3070.800178
Internal Thermal Energy = -3070.788859
Enthalpy = -3070.787915
Gibbs Free Energy = -3070.840233

C,0,-0.5419940015,-0.8680323532,-0.5858766811
C,0,-0.1816941703,-1.5247596261,-1.8754419108
C,0,-0.3259618305,2.6540894187,0.4916628016
C,0,-0.3999316672,1.1471961007,0.6359956053
O,0,-0.3356697101,0.5571157874,1.6916493869
O,0,-0.5492327209,0.5597772296,-0.5738625779

C,0,0.7634088651,-1.6022780845,-0.6668936412
O,0,0.8636424879,-2.7630253941,0.1110250795
O,0,-0.9773156394,-2.6143893975,-2.2550984961
Br,0,1.5445132596,3.1566680719,0.0265957325
H,0,-1.3245132716,-1.3263763205,0.0141229481
H,0,0.1597115599,-0.8778587108,-2.6860681965
H,0,-0.9504845007,3.0303213852,-0.3183461606
H,0,-0.5451376643,3.1382166211,1.4414234001
H,0,1.6706241025,-1.0002396874,-0.7490605857
H,0,1.3891137945,-3.4072353433,-0.3819442169
H,0,-0.4158498931,-3.2385136973,-2.7339444872

TS–diOHCPr-Bromoacetate

E (total electronic) = -3070.8933327
E (total electronic)+ZPVE = -3070.775752
Internal Thermal Energy = -3070.764479
Enthalpy = -3070.763535
Gibbs Free Energy = -3070.816938

C,0,-0.6238980674,-1.2270287522,-0.8442528815
C,0,-0.8931695835,-1.8689631625,-2.0817750996
C,0,0.6430969467,-1.8700523624,-0.8090981202
O,0,1.013050769,-2.5535534293,0.3015699796
O,0,-2.0565794152,-2.5502095826,-2.2357924295
H,0,-1.2905007603,-1.5046674653,-0.0301169474
H,0,-0.2921669266,-1.6965842045,-2.9697269609
H,0,1.4034463169,-1.6922455706,-1.5641834384
H,0,1.8333004829,-3.0340002673,0.1237862422
H,0,-2.0324287227,-3.0439380192,-3.0671753502
C,0,-0.5551652844,2.5785332115,0.2756173997
C,0,-0.6236402514,1.0500050257,0.3622578372
O,0,-0.5731631433,0.4774614112,1.4473163036
O,0,-0.7348642912,0.4889575326,-0.8174699593
Br,0,1.3467088496,3.1286491003,0.0107515654
H,0,-1.0976692744,2.980337495,-0.5802530258
H,0,-0.8671606444,3.0375560395,1.2133318847

diOHCPr-Dichloroacetate

E (total electronic) = -1415.3412974
E (total electronic)+ZPVE = -1415.231290
Internal Thermal Energy = -1415.218835
Enthalpy = -1415.217890
Gibbs Free Energy = -1415.272895

C,0,-0.4137227124,-0.91313839,-0.3098798583
C,0,0.1427973165,-1.6183445988,-1.4995103357
C,0,-0.4485072723,2.6822087965,0.6510888596
C,0,-0.4743857228,1.1523237186,0.8160018489
O,0,-0.528916825,0.6384219608,1.9087081701
O,0,-0.4313488264,0.5173900987,-0.3621219596
C,0,0.8913004946,-1.6350689154,-0.157520387
O,0,0.8726598171,-2.7579430792,0.6784588115
O,0,-0.5834930946,-2.7283071036,-1.9493046601
Cl,0,-1.8911166775,3.2542178159,-0.2570640333
Cl,0,1.0897366102,3.2104653394,-0.1170075258
H,0,-1.2794229304,-1.3489916442,0.1826969453
H,0,0.6034180884,-1.0014628747,-2.2737085458
H,0,-0.4880684313,3.1398408079,1.6376943715
H,0,1.798367932,-1.0281612113,-0.1273245504
H,0,1.4650894811,-3.4209048759,0.2995316141
H,0,0.0450277528,-3.3675648443,-2.310482765

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3185968
E (total electronic)+ZPVE = -1415.209873
Internal Thermal Energy = -1415.197608
Enthalpy = -1415.196664
Gibbs Free Energy = -1415.251831

C,0,-1.8299554954,0.2226847158,0.0913683123
C,0,-2.6797283344,0.998592006,-0.742737786
C,0,-2.5431594448,-0.9159477926,-0.3769048037
O,0,-3.0769531784,-1.7814008331,0.5233332382
O,0,-3.349592701,2.0520676615,-0.2053797023
C,0,2.1163714795,-0.1951680237,0.4149127385
C,0,0.5937304252,-0.2659020843,0.7244298353
O,0,0.2384336746,-0.9097908588,1.7027711519
O,0,-0.1470263763,0.3769511833,-0.1297411499
Cl,0,2.7088049118,1.5063782608,0.3547630052
Cl,0,2.4813507724,-1.0802099545,-1.1155631808
H,0,-1.940411425,0.4129615935,1.1573193748
H,0,-2.6618512895,0.9169183312,-1.8255485343
H,0,-2.5039113475,-1.2348895652,-1.4142753353
H,0,-3.6319974969,-2.4226265377,0.0586706303
H,0,-3.9856921855,2.3885891659,-0.8512397278
H,0,2.6728080111,-0.6945212682,1.2063389338

diOHCPr-Trifluoroacetate

E (total electronic) = -793.7610103
E (total electronic) + ZPVE = -793.656087
Internal Thermal Energy = -793.643785
Enthalpy = -793.642841
Gibbs Free Energy = -793.696751

C,0,-0.7903953919,-0.1752975432,-0.4166815364
C,0,-1.9781190978,-0.7958425007,0.2344561981
C,0,2.8440763593,-0.6631592138,0.1857026289
C,0,1.5468762929,0.073604449,-0.2988860509
O,0,1.5573204323,1.1678667696,-0.7986132133
O,0,0.4939073436,-0.7113002908,-0.0604257873
C,0,-1.5554538282,0.6407729235,0.5814652908
O,0,-2.2339554294,1.7506468938,0.0660045377
O,0,-3.0663214218,-1.0596886155,-0.6055867308
F,0,3.9277797248,0.0917250506,-0.0423696179
F,0,3.0030348273,-1.8378074585,-0.4626253199
F,0,2.7800013915,-0.921325841,1.5106581579
H,0,-0.8701908975,0.1140913396,-1.4612698926
H,0,-1.7887658836,-1.5296196832,1.0203624474
H,0,-1.1136755715,0.7635559844,1.5722804705
H,0,-3.0664760419,1.8417140168,0.5487184084
H,0,-3.8742568078,-0.9554712808,-0.0854729906

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.7405241

E (total electronic) + ZPVE = -793.636972
Internal Thermal Energy = -793.624816
Enthalpy = -793.623872
Gibbs Free Energy = -793.678049

C,0,-1.0403957488,-0.5032123759,-0.3207504168
C,0,-2.2357951569,-1.1535542742,0.0920164245
C,0,-1.5434413649,0.6171286204,0.3998704356
O,0,-1.6413991603,1.8180716352,-0.2294766327
O,0,-3.0298130689,-1.7325162463,-0.8488862951
H,0,-0.9537863955,-0.3449455139,-1.3940543626
H,0,-2.4284241475,-1.4030192987,1.1312715771
H,0,-1.6368565837,0.6105726375,1.4818793845
H,0,-2.1131196765,2.4390352826,0.3421581262
H,0,-3.8603595745,-2.0090998675,-0.4381770001
C,0,2.8086428826,-1.3484153004,0.1153973039
C,0,1.5018608643,-0.6186705373,-0.3873690123
O,0,1.5798394421,0.3761414604,-1.0840164923
O,0,0.4486330907,-1.2353379058,0.0600667207
F,0,2.8353761427,-2.6410491712,-0.2922326293
F,0,3.9231253302,-0.7531199521,-0.348200502
F,0,2.8742551248,-1.3440381928,1.4698313709

diOHCPr-Trichloroacetate
E (total electronic) = -1874.9633279
E (total electronic)+ZPVE = -1874.863657
Internal Thermal Energy = -1874.849988
Enthalpy = -1874.849044
Gibbs Free Energy = -1874.906796

C,0,-0.9403472093,-0.0052180142,-0.6394484794
C,0,-2.1241073704,-0.6340746542,0.0109790916
C,0,2.7035483723,-0.4874227193,-0.0092822475
C,0,1.3922055706,0.2401620726,-0.4974488632
O,0,1.3795535527,1.3539995421,-0.9506252318
O,0,0.340316695,-0.5612447704,-0.3100539689
C,0,-1.6873799107,0.7908559544,0.3880044977
O,0,-2.3669486307,1.9167737782,-0.0904373657
O,0,-3.2259873498,-0.8688990643,-0.8200554241
Cl,0,4.130178669,0.5182185868,-0.3563415609
Cl,0,2.8721652486,-2.0696392563,-0.8473371683
Cl,0,2.5654771621,-0.7384389563,1.7713648883
H,0,-1.0303130936,0.3105576444,-1.6756491092
H,0,-1.9297365925,-1.3888475761,0.775491158
H,0,-1.2315104064,0.886847804,1.3754600939
H,0,-3.2012292235,1.9893576254,0.3923489434
H,0,-4.0253744833,-0.7763799968,-0.2847462536

TS–diOHCPr-Trichloroacetate
E (total electronic) = -1874.9429518
E (total electronic)+ZPVE = -1874.844707
Internal Thermal Energy = -1874.831135
Enthalpy = -1874.830190
Gibbs Free Energy = -1874.888832

C,0,2.2321644342,0.0606449768,-0.2060834651
C,0,3.2518045843,0.9060931223,0.3119380984
C,0,2.8772502696,-0.9697425608,0.5362072237
O,0,3.2482551962,-2.1117133081,-0.1007925659
O,0,3.9963312843,1.6465683001,-0.5529009643
H,0,2.2593840849,-0.0793452785,-1.2851421072
H,0,3.3143541205,1.1559409831,1.3668826674
H,0,2.8837726597,-0.9781357206,1.6221608667
H,0,3.7819475969,-2.6508729448,0.4986928178
H,0,4.7276804256,2.0575124349,-0.0720756354
C,0,-1.7388781437,0.1055389386,0.0189779046
C,0,-0.2643263567,-0.3138090148,-0.4357513049
O,0,-0.0893756582,-1.29064643,-1.1363263089
O,0,0.6167748872,0.4966297565,0.0671509335
Cl,0,-2.0438331626,1.8375039731,-0.376382391
Cl,0,-2.977683051,-0.8973215428,-0.7938123906
Cl,0,-1.8601401411,-0.1438789451,1.8055085113

diOHCPr-Heptafluorobutanoate
E (total electronic) = -1269.2602552
E (total electronic)+ZPVE = -1269.131856
Internal Thermal Energy = -1269.113943
Enthalpy = -1269.112999
Gibbs Free Energy = -1269.179428

C,0,2.4482689519,-0.5304211131,0.1106143557
C,0,3.2950198105,-0.0036640002,-0.9959616687
C,0,2.8491564492,0.9130469289,0.1555332582
O,0,3.7181766504,1.2688633164,1.1924915445
O,0,4.5942653083,-0.5186551201,-1.0685046439
C,0,-1.2052052834,-1.244400042,0.2326754005
F,0,-1.1490567894,-2.3551557869,-0.5551245642
C,0,0.2257928364,-0.9104029502,0.7851273914
O,0,0.4414785885,-0.717396563,1.952772609
O,0,1.09549508,-0.8808628318,-0.2248802271
F,0,-2.0221144736,-1.5105886176,1.277233999
C,0,-1.8750563904,-0.1036282602,-0.6348784843
C,0,-1.9841123142,1.2981373478,0.0732639158
F,0,-3.1276355073,-0.5024320168,-0.9642787593
F,0,-1.1608980894,0.0639787929,-1.7721229176
F,0,-2.7098095548,1.215560765,1.1959260667
F,0,-2.5656985014,2.1764050835,-0.7554933178
F,0,-0.7532046513,1.7493560987,0.3836452066
H,0,2.906176693,-1.1975282988,0.8361104288
H,0,2.8013754876,0.1924536184,-1.9498632706
H,0,2.0935271784,1.6526205957,-0.1143625208
H,0,4.3091811115,1.9585954603,0.8617901152
H,0,5.1696384095,0.176180593,-1.4153939168

TS–diOHCPr-Heptafluorobutanoate
E (total electronic) = -1269.2401476
E (total electronic)+ZPVE = -1269.113357
Internal Thermal Energy = -1269.095490
Enthalpy = -1269.094546
Gibbs Free Energy = -1269.161715

C,0,0.9467865933,2.1509507932,-0.4880265308
F,0,-0.243882818,2.7832087021,-0.2589377252

C,0,0.8079874644,0.6041339862,-0.1930935441
O,0,1.6332641826,0.0443891515,0.5041497235
O,0,-0.2286179635,0.1120707106,-0.8008371667
F,0,1.8661220382,2.6976246475,0.3484496107
C,0,1.3692090052,2.5100407116,-1.9657706092
C,0,2.6861667589,1.8141940497,-2.4746795229
F,0,1.5550856804,3.8534984565,-2.0493969402
F,0,0.3717608899,2.1638113669,-2.8142426142
F,0,3.7285778715,2.1201680399,-1.6890935593
F,0,2.9558107762,2.2217528964,-3.7252995039
F,0,2.5289377382,0.4776756641,-2.4861494942
C,0,-0.3358198639,-1.5851879382,-0.7762535163
C,0,-1.3868925063,-2.2036918217,-1.5078879916
C,0,0.5236458329,-2.4051233411,-1.5621517505
O,0,1.4284031447,-3.2044560383,-0.9376196113
O,0,-2.4018082362,-2.8011296965,-0.8267058922
H,0,-0.3243442189,-1.8088830306,0.288589719
H,0,-1.5331772671,-2.0262064978,-2.5691918039
H,0,0.6457693612,-2.2505716706,-2.6301209105
H,0,1.849102323,-3.7797472157,-1.5909986801
H,0,-2.9589807869,-3.2888009256,-1.4486796862

M06-2X/AUG-cc-pVTZ
SMD, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.9106332
E (total electronic) + ZPVE = -456.804351
Internal Thermal Energy = -456.796052
Enthalpy = -456.795108
Gibbs Free Energy = -456.837621

C,0,-0.8240015093,-0.2654612158,-0.3852358209
C,0,-1.9985309744,-0.837609607,0.3178755689
C,0,1.4710015762,0.0369472492,-0.1377259117
O,0,1.394504038,1.1808720111,-0.501822968
O,0,0.4381636125,-0.803053018,-0.0473317872
C,0,-1.543142967,0.5714791414,0.6138653069
O,0,-2.2595281976,1.6537617357,0.0946201321
O,0,-3.1388893074,-1.0432404234,-0.4645874663
H,0,-0.9424654661,0.0017851287,-1.4268036982
H,0,-1.8059865135,-1.5732742784,1.0886795843
H,0,-1.0589789349,0.7286917566,1.5702617659
H,0,-3.1039558834,1.7117484256,0.5574268466
H,0,-3.9123423982,-0.7949100647,0.0559792165
H,0,2.3952234052,-0.4625164872,0.1607696012

TS–diOHCPr-Formate
E (total electronic) = -456.8602364
E (total electronic) + ZPVE = -456.757308
Internal Thermal Energy = -456.748843
Enthalpy = -456.747899
Gibbs Free Energy = -456.791231

C,0,-1.1893091679,-0.1615570794,-0.1791882978
C,0,-2.3128854713,-0.851129733,0.2769239559
C,0,-1.6561744234,0.9734735476,0.483962911
O,0,-1.7181225961,2.1467564004,-0.1686592791
O,0,-3.0565712401,-1.5619581868,-0.5910368424
H,0,-1.0624654539,-0.0835778157,-1.2504891298
H,0,-2.5424901068,-0.9574191576,1.3269134689
H,0,-1.8387700589,0.9888681655,1.5483775336
H,0,-2.1353396706,2.8138657339,0.3914211318
H,0,-3.8494651572,-1.8957395913,-0.1517707347
C,0,1.4239671929,-0.0560814552,0.0083742619
O,0,1.3439056539,1.0597197315,-0.5064599481
O,0,0.4546427249,-0.8694551055,0.2098864535
H,0,2.4022900245,-0.4333455945,0.3471355653

diOHCPr-Acetate
E (total electronic) = -496.2313635
E (total electronic) + ZPVE = -496.097418
Internal Thermal Energy = -496.087598
Enthalpy = -496.086653
Gibbs Free Energy = -496.132653

C,0,-0.8226218248,-0.275925688,-0.3731529479
C,0,-2.0051096903,-0.8324410711,0.329974379
C,0,2.7561170152,-0.6579933006,0.2732406219
C,0,1.4878107247,0.0092799002,-0.135811033
O,0,1.3792001688,1.1452171816,-0.5326913005
O,0,0.4302605395,-0.8184914215,-0.0219658461
C,0,-1.54442611,0.5775523467,0.6103163064
O,0,-2.2573078838,1.655463917,0.076604084
O,0,-3.1416206975,-1.041960342,-0.4578783221
H,0,-0.9380114995,-0.0230099496,-1.4188576504
H,0,-1.8224867589,-1.5602980401,1.110926088
H,0,2.6560205271,-1.0372112052,1.2890855541
H,0,2.9394489591,-1.5074086738,-0.3840291034
H,0,-1.0655867968,0.7448802619,1.5676329233
H,0,-3.094905215,1.7297977015,0.5495410381
H,0,-3.9169908329,-0.7863553184,0.0559231613
H,0,3.5787218649,0.0461716013,0.2112335471

TS–diOHCPr-Acetate
E (total electronic) = -496.1780071
E (total electronic) + ZPVE = -496.047146
Internal Thermal Energy = -496.037277
Enthalpy = -496.036333
Gibbs Free Energy = -496.082920

C,0,-0.6782219902,-1.0110077994,-0.6793771928
C,0,-0.8776478486,-1.5060449011,-1.9671752161
C,0,0.5359660114,-1.6925517889,-0.6079353912
O,0,0.8161079976,-2.4394184414,0.4719284181
O,0,-2.0589394207,-2.0609320818,-2.2905163722
C,0,-0.3389004832,2.7189891077,0.8665628364
C,0,-0.3835030967,1.2199790889,0.7030987187
O,0,-0.0667012475,0.4670077681,1.6327181137
O,0,-0.7515431594,0.8101034791,-0.4626719202
H,0,-1.4228584104,-1.2624691039,0.0635645522
H,0,-0.1687487696,-1.3506250185,-2.7673539247
H,0,1.3283723291,-1.5456613244,-1.3274171303
H,0,1.6438114129,-2.9190242071,0.3390529954
H,0,-2.0166990854,-2.4383066992,-3.1784183351
H,0,0.4757288403,3.1113868043,0.2571115781
H,0,-1.2653547068,3.1624105839,0.5063931408
H,0,-0.1734093726,2.9875705338,1.9058731294

diOHCPr-2,2-Dimethylpropanoate
E (total electronic) = -614.1554088
E (total electronic) + ZPVE = -613.936948
Internal Thermal Energy = -613.923079
Enthalpy = -613.922135
Gibbs Free Energy = -613.977729

C,0,-1.3307937063,-0.1964208882,-0.4023932046
C,0,-2.41621217,-0.8714122326,0.3507242093
C,0,2.3181058006,-0.134269405,0.0892976694
C,0,0.9360705534,0.3623118803,-0.2815735662
O,0,0.6698077198,1.4598250481,-0.7117443931
O,0,-0.0115067138,-0.5731335672,-0.0844956888
C,0,-2.123506377,0.59252219,0.5793724334

O,0,-2.9722358108,1.5619288972,0.0361086148
O,0,-3.5375756389,-1.2447453945,-0.3972594413
C,0,2.6458728112,-1.3594080493,-0.7714808222
C,0,3.3319688301,0.9734651547,-0.1670111324
C,0,2.3196431684,-0.52012176,1.5724831022
H,0,-1.5096170101,0.0114266109,-1.4491887074
H,0,-2.1250566713,-1.5460437248,1.1464753227
H,0,-1.6451174667,0.8442174403,1.5183833429
H,0,-3.7986229911,1.556113349,0.5335255675
H,0,-4.3253775827,-1.0815847223,0.1347638783
H,0,3.6574648856,-1.6916256076,-0.5366149319
H,0,1.9589257738,-2.1804557488,-0.5730995778
H,0,2.602784233,-1.1143719854,-1.8334874479
H,0,3.1156320632,1.8539619682,0.4377792212
H,0,4.326650431,0.6119671888,0.0933102293
H,0,3.33570672,1.2684257707,-1.2162083373
H,0,3.3235217003,-0.8431242802,1.849510952
H,0,2.0488220048,0.3312907358,2.1984119357
H,0,1.6275238034,-1.3366150675,1.7721273981

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.1017552
E (total electronic) + ZPVE = -613.886646
Internal Thermal Energy = -613.872659
Enthalpy = -613.871715
Gibbs Free Energy = -613.928883

C,0,-1.7299840887,-0.1143806081,-0.1676807598
C,0,-2.7255788773,-0.9513007531,0.3332473107
C,0,-2.2816336339,0.9600176849,0.5285308577
O,0,-2.4924859608,2.1247866507,-0.1042516629
O,0,-3.3935023629,-1.7677751513,-0.5004555262
H,0,-1.6625278523,-0.0163213385,-1.242716497
H,0,-2.903748459,-1.0731998911,1.3916728891
H,0,-2.4330198906,0.9427731193,1.5979310562
H,0,-2.9541841208,2.7408532301,0.4787916954
H,0,-4.1087580756,-2.2118003487,-0.0272320575
C,0,2.345408893,-0.1663470772,0.0507366923
C,0,0.8903867863,0.2461163715,-0.2080684448
O,0,0.6088722036,1.350202134,-0.6892588308
O,0,0.0073054466,-0.6352118851,0.1146147108
C,0,3.3016596079,0.933682526,-0.3924489758
C,0,2.6344761644,-1.4487306925,-0.7342743405
C,0,2.5172593985,-0.4261201771,1.5497720053
H,0,4.328270654,0.618963546,-0.1996880489
H,0,3.2019880855,1.1398448907,-1.4582158181
H,0,3.1210560108,1.8599899972,0.152985581
H,0,3.6759873297,-1.738219781,-0.5861531978
H,0,1.9993342603,-2.268249446,-0.4005951823
H,0,2.4711352137,-1.2967672364,-1.8028150765
H,0,3.554149075,-0.6980242555,1.7536393337
H,0,2.2800484288,0.4666060592,2.1313839244
H,0,1.8767277638,-1.2401675678,1.8867153624

diOHCPr-Fluoroacetate

E (total electronic) = -595.4737539
E (total electronic) + ZPVE = -595.346826
Internal Thermal Energy = -595.336281
Enthalpy = -595.335337
Gibbs Free Energy = -595.383904

C,0,0.2659576722,-0.9473538989,-0.213522998
C,0,0.8743224678,-1.47840916,1.0304287119
C,0,-0.8575599514,2.4249619327,-1.033107183
C,0,-0.8503239122,0.9202814685,-1.0481877516
O,0,-1.6419258224,0.2282418845,-1.6314861982
O,0,0.1666622868,0.4581579763,-0.3154656531
C,0,-0.6005905946,-1.6619986602,0.7632811075
O,0,-1.0795462661,-2.9096780756,0.3543405446
O,0,1.7451233348,-2.5597642246,0.866465807
F,0,-1.8784494381,2.8819160995,-1.8336322377
H,0,0.4915552719,-1.4565480279,-1.1408709006
H,0,1.1350997894,-0.7634967438,1.8010214143
H,0,-1.0135894807,2.7757530402,-0.013345974
H,0,0.0929649293,2.7992768571,-1.4107247434
H,0,-1.2736971015,-1.0600367988,1.3618552016
H,0,-1.0436953748,-3.5106955566,1.1082897028
H,0,1.6036301895,-3.1751551123,1.5956891502

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.425241
E (total electronic) + ZPVE = -595.301250
Internal Thermal Energy = -595.290748
Enthalpy = -595.289803
Gibbs Free Energy = -595.338858

C,0,-0.0755861837,-1.294509556,-0.0412995704
C,0,-0.9942183485,-1.8101848366,-0.9562668489
C,0,0.9432418091,-1.8697984124,-0.8021273394
O,0,1.88074118,-2.6189653949,-0.1950477036
O,0,-2.0610375719,-2.5003901591,-0.5103744461
H,0,-0.1652359778,-1.6307561516,0.9829425505
H,0,-0.971924228,-1.5598033436,-2.0067499897
H,0,1.1034703642,-1.6220641008,-1.8411754633
H,0,2.4615685028,-3.0203333711,-0.8539331828
H,0,-2.5501905301,-2.8702071041,-1.2563897469
C,0,0.9040189819,2.4311788781,1.0891764669
C,0,0.9017956747,0.9214155797,0.9449838061
O,0,1.8000755312,0.2325485811,1.4219845666
O,0,-0.1130179556,0.4933440839,0.2836645265
F,0,2.0100602146,2.8562475532,1.8030728663
H,0,0.9300131853,2.8892967785,0.1014667929
H,0,0.0066313517,2.7487979757,1.6180877153

diOHCPr-Chloroacetate

E (total electronic) = -955.8352442
E (total electronic) + ZPVE = -955.710231
Internal Thermal Energy = -955.699262
Enthalpy = -955.698318
Gibbs Free Energy = -955.748552

C,0,-0.1010068713,-1.0462877313,0.3589526706
C,0,-0.8329372568,-1.8145526545,-0.6771544767
C,0,0.5671726951,2.5236550089,0.5953506994

C,0,0.8330143522,1.0504907131,0.761121492
O,0,1.8227799901,0.5440717187,1.2155278003
O,0,-0.2227900169,0.3601917813,0.3102647559
C,0,0.6759420235,-1.7417339717,-0.7020543636
O,0,1.4336319345,-2.8376198921,-0.2796448744
O,0,-1.4632769167,-2.9809669589,-0.2335575076
Cl,0,1.8814515601,3.5144825808,1.2512824473
H,0,-0.0584516398,-1.4649047866,1.3556142767
H,0,-1.3500209977,-1.2502054688,-1.4433799816
H,0,0.4578978205,2.7448851605,-0.4633157139
H,0,-0.3550488419,2.7813449191,1.1082373132
H,0,1.1106593013,-1.1273490695,-1.4813030571
H,0,1.3999932275,-3.5137868392,-0.9667896352
H,0,-1.3887003638,-3.6474455098,-0.926847845

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.7866509
E (total electronic) + ZPVE = -955.664304
Internal Thermal Energy = -955.653509
Enthalpy = -955.652564
Gibbs Free Energy = -955.702789

C,0,-0.0704533893,-1.3325761211,-0.1722255439
C,0,-0.9941248582,-1.8397418974,-1.0869687127
C,0,0.9458388328,-1.9022168177,-0.9406399364
O,0,1.8851590171,-2.6567921712,-0.3433496109
O,0,-2.059889908,-2.5312918536,-0.64114768
H,0,-0.1566864022,-1.676078438,0.8498704574
H,0,-0.9753058973,-1.582765643,-2.1359871012
H,0,1.1015779679,-1.6474190128,-1.9786572928
H,0,2.4650901391,-3.0510710531,-1.0073723573
H,0,-2.5529836959,-2.8956765727,-1.3872820817
C,0,0.9065826635,2.3795164171,0.978793061
C,0,0.9108530687,0.8636143846,0.847835187
O,0,1.7832066588,0.1531894438,1.3344589794
O,0,-0.0993095839,0.452952793,0.1644801132
Cl,0,2.279870495,3.0209514264,1.9181147488
H,0,0.9449679442,2.8210348266,-0.0126493
H,0,-0.0088360523,2.6930312893,1.4716740697

diOHCPr-Bromoacetate

E (total electronic) = -3069.8693752
E (total electronic)+ZPVE = -3069.744845
Internal Thermal Energy = -3069.733788
Enthalpy = -3069.732844
Gibbs Free Energy = -3069.783784

C,0,-0.1564027315,-1.0869214915,0.3635219961
C,0,-0.8980020627,-1.8525734935,-0.6677109005
C,0,0.5193135498,2.4797016813,0.5858888694
C,0,0.7803839309,1.007968416,0.7707974564
O,0,1.7637559072,0.4960661331,1.2304752547
O,0,-0.2793588878,0.3195131596,0.3195685103
C,0,0.6105151133,-1.7774515009,-0.7079375649
O,0,1.3738511336,-2.8745140087,-0.2988490759
O,0,-1.5210592828,-3.0219857652,-0.2214515009
Br,0,1.90226034,3.5853264112,1.347282007
H,0,-0.1034824561,-1.5089634448,1.3582314378
H,0,-1.4245409877,-1.2869908827,-1.4265647824
H,0,0.457962542,2.6935848809,-0.4780062129
H,0,-0.4256704752,2.7416783697,1.0517849613
H,0,1.0361744741,-1.1591340686,-1.4890990247
H,0,1.3331976031,-3.5473895311,-0.9888546904
H,0,-1.4503117105,-3.6869928646,-0.9165717403

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.8203993
E (total electronic)+ZPVE = -3069.698738
Internal Thermal Energy = -3069.687727
Enthalpy = -3069.686782
Gibbs Free Energy = -3069.738384

C,0,-0.0694760017,-1.3670814238,-0.2088712391
C,0,-0.9959962135,-1.8532608779,-1.131840251
C,0,0.9472994798,-1.9353523037,-0.9775439365
O,0,1.8793994448,-2.700597182,-0.3833092568
O,0,-2.0730614524,-2.5345357473,-0.6990302267
H,0,-0.1625621741,-1.7187315872,0.8098717991
H,0,-0.9672803033,-1.5880291507,-2.1786081908
H,0,1.1076898052,-1.6740829817,-2.0132976158
H,0,2.461042142,-3.0910225298,-1.0481711381
H,0,-2.5677824958,-2.8827238175,-1.4518629899
C,0,0.9069603481,2.3499334181,0.9246001944
C,0,0.9251840432,0.8315797154,0.8159403421
O,0,1.7970139207,0.124358696,1.3042991824
O,0,-0.0911582828,0.4163640192,0.1405285267
Br,0,2.4034519827,3.1157517753,1.8889294376
H,0,0.911559935,2.777937843,-0.0728125696
H,0,0.0011968217,2.6594701344,1.4365889321

diOHCPr-Dichloroacetate

E (total electronic) = -1415.4333311
E (total electronic)+ZPVE = -1415.317380
Internal Thermal Energy = -1415.305561
Enthalpy = -1415.304617
Gibbs Free Energy = -1415.357505

C,0,1.6594122086,-0.327688612,-0.5225439838
C,0,2.7274775956,0.7012279883,-0.5256846509
C,0,-1.952058924,0.2073822842,-0.4848371307
C,0,-0.632509684,-0.4909450139,-0.1783804403
O,0,-0.5044712831,-1.4246397322,0.5610294992
O,0,0.3524506714,0.1211127002,-0.8278238688
C,0,2.2678221758,0.0791965851,0.7719749391
O,0,3.0575420905,-0.8870673575,1.3997401323
O,0,3.9434410231,0.3088396695,-1.0912349737
Cl,0,-2.0228292905,1.646348023,0.564295267
Cl,0,-3.32057017,-0.8608477112,-0.1948602144
H,0,1.8997310755,-1.311819061,-0.9013578821
H,0,2.4262375147,1.7279770723,-0.6936400801
H,0,-1.9831369005,0.5456922411,-1.5135430494
H,0,1.6715819328,0.7121965027,1.4192597009
H,0,3.8177072566,-0.4468401411,1.7988160819
H,0,4.6580067075,0.6979045626,-0.5731663461

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3887412
E (total electronic)+ZPVE = -1415.275632
Internal Thermal Energy = -1415.263816
Enthalpy = -1415.262872
Gibbs Free Energy = -1415.316822

C,0,-0.5016859252,-1.3909816889,-0.6405384733
C,0,0.2175695374,-2.0686767585,-1.6279031807
C,0,0.5133141219,-1.7730666711,0.2414104737
O,0,0.1892480301,-2.3837577507,1.3979391628
O,0,-0.4079073156,-2.9797581863,-2.4011909487
H,0,-1.4972774523,-1.7528522975,-0.4213794431
H,0,1.2175243048,-1.7788346222,-1.9141755939
H,0,1.5390362051,-1.4583326733,0.1160815633
H,0,0.9907288273,-2.6543757852,1.863435326
H,0,0.2324221701,-3.4168247237,-2.9770936924
C,0,-0.6644123371,2.5385035191,-0.142324238
C,0,-0.8677347187,1.0419820838,0.1539385404
O,0,-0.9326387323,0.6320246991,1.3025192952
O,0,-0.8921607455,0.3449104501,-0.9185975991
Cl,0,-1.3748251821,3.5725577405,1.1027089291
Cl,0,1.0991403919,2.801951953,-0.2543111753
H,0,-1.0931901798,2.8158627116,-1.096261946

diOHCPr-Trifluoroacetate

E (total electronic) = -793.9852064
E (total electronic) + ZPVE = -793.874655
Internal Thermal Energy = -793.862705
Enthalpy = -793.861761
Gibbs Free Energy = -793.914921

C,0,-0.7818978287,-0.2360230987,-0.4542757006
C,0,-1.9483947644,-0.793711531,0.2694526482
C,0,2.8071976249,-0.6463091368,0.1894179685
C,0,1.507395337,0.0608628958,-0.2437784107
O,0,1.4870579478,1.1877312051,-0.6409013328
O,0,0.487830172,-0.7632434311,-0.1062729157
C,0,-1.4951931761,0.6241270784,0.5280178147
O,0,-2.2102136549,1.6931485777,-0.0159669906
O,0,-3.0849394184,-1.0292724951,-0.5075459537
F,0,3.8329526311,0.187435651,0.1200033603
F,0,3.0575746557,-1.6896782397,-0.5998552777
F,0,2.7072134902,-1.0904725788,1.4405889647
H,0,-0.8942688339,-0.0006977534,-1.5037488363
H,0,-1.7464713616,-1.5068304887,1.0592310466
H,0,-1.0070308929,0.801733224,1.4788233925
H,0,-3.0417842286,1.7783376995,0.4657462246
H,0,-3.8616416995,-0.7826725783,0.008780998

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.9443793
E (total electronic) + ZPVE = -793.836271
Internal Thermal Energy = -793.824478
Enthalpy = -793.823534
Gibbs Free Energy = -793.876546

C,0,-1.1030881021,-0.5798730678,-0.4056336132
C,0,-2.2653239747,-1.1427861337,0.1285102582
C,0,-1.4824521218,0.5776113281,0.2814396643
O,0,-1.5467519189,1.7479435837,-0.3863354539
O,0,-3.1459750428,-1.7520791493,-0.6940262696
H,0,-1.0454825716,-0.505811299,-1.483646948
H,0,-2.4103575263,-1.2704962497,1.1906605489
H,0,-1.5533546854,0.6165513106,1.3582703683
H,0,-1.8981454591,2.4365599809,0.192068972
H,0,-3.934472675,-2.0079492505,-0.198744182
C,0,2.8025619865,-1.3013813176,0.1163436962
C,0,1.4678874469,-0.6160012636,-0.2763791291
O,0,1.491433236,0.5335446654,-0.6776673117
O,0,0.4717948644,-1.391909614,-0.1145822353
F,0,3.0199820561,-2.3838121762,-0.637873887
F,0,3.8415323182,-0.4861746494,-0.0350488038
F,0,2.7785541696,-1.6999656979,1.3919723257

diOHCPr-Trichloroacetate

E (total electronic) = -1875.0247406
E (total electronic)+ZPVE = -1874.919584
Internal Thermal Energy = -1874.906407
Enthalpy = -1874.905463
Gibbs Free Energy = -1874.962497

C,0,-1.3058557868,-0.1882299006,-0.4307498473
C,0,-2.3623504293,-0.9068908068,0.3198869855
C,0,2.3402538968,-0.1329687144,0.0761850814
C,0,0.9273496236,0.4050748396,-0.2588893247
O,0,0.7163869685,1.5358941979,-0.5809242396
O,0,0.032436292,-0.5608595083,-0.151266021
C,0,-2.0775628353,0.5490505476,0.6054746011
O,0,-2.94012266,1.5355338548,0.1229267377
O,0,-3.4933213694,-1.2618946655,-0.4191246718
H,0,-1.4928729255,0.0608060191,-1.4664857744
H,0,-2.0403933313,-1.6099782336,1.0782688317
H,0,-1.573659272,0.7614329894,1.5411739391
H,0,-3.7560948361,1.5045956425,0.6367028079
H,0,-4.2693886023,-1.1495525774,0.1428129264
Cl,0,3.5070723741,1.1828071058,0.0551649771
Cl,0,2.3152649174,-0.8860883414,1.6795458828
Cl,0,2.7678903156,-1.3355838185,-1.1571696819

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1874.9835708
E (total electronic)+ZPVE = -1874.881060
Internal Thermal Energy = -1874.868009
Enthalpy = -1874.867065
Gibbs Free Energy = -1874.923454

C,0,2.2979308533,0.1388595902,-0.3466868637
C,0,3.25898896,0.920845235,0.29938392
C,0,2.7732699648,-0.9108349588,0.4461161495
O,0,3.1341904582,-2.0699945275,-0.1417680983
O,0,4.1241729153,1.6506625818,-0.4361278923

H,0,2.3987952954,0.0225512578,-1.4176174532
H,0,3.2348527785,1.1063101237,1.3627585412
H,0,2.7036390821,-0.9012049622,1.5238149005
H,0,3.5267974514,-2.661802649,0.5124292448
H,0,4.7756058506,2.0677451699,0.1419748254
C,0,-1.6877754042,0.047783522,0.0416343353
C,0,-0.2294947945,-0.3039013487,-0.4208920831
O,0,0.0037344939,-1.4413096737,-0.785828693
O,0,0.5845728674,0.6631862098,-0.285667522
Cl,0,-2.1110935171,1.7262857436,-0.3227962962
Cl,0,-2.8715665774,-1.0249109947,-0.7108444412
Cl,0,-1.7011376477,-0.1993035792,1.8083693162

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.6066249
E (total electronic)+ZPVE = -1269.471068
Internal Thermal Energy = -1269.453475
Enthalpy = -1269.452531
Gibbs Free Energy = -1269.519981

C,0,-2.3288685826,-0.5414837011,0.4522179705
C,0,-3.135392672,0.6841422892,0.6587303924
C,0,-2.813196256,0.2081693942,-0.7381443267
O,0,-3.7911076354,-0.4428364432,-1.4930212499
O,0,-4.4140619174,0.4880845166,1.1847860174
C,0,1.3264789879,-1.0257627048,0.5517927549
F,0,1.386016293,-0.6442525025,1.8346079614
C,0,-0.1336332919,-1.1807549438,0.0732260973
O,0,-0.4036535583,-1.868795818,-0.8670372515
O,0,-0.9582139897,-0.4729327228,0.816010202
F,0,1.9341116721,-2.2169975203,0.4323127347
C,0,2.1632625586,-0.030801799,-0.2891092653
C,0,1.6261008967,1.4134934289,-0.3439069733
F,0,2.2331810062,-0.4876813728,-1.545944916
F,0,3.3971731935,0.0081400037,0.2291608237
F,0,0.4306932862,1.4258702436,-0.9241661181
F,0,2.4550230569,2.1596616012,-1.0576901723
F,0,1.5226197434,1.9256403627,0.872531854
H,0,-2.7893557785,-1.4979392345,0.6582784926
H,0,-2.6078090408,1.5721525805,0.9857407713
H,0,-2.0932905842,0.8004922117,-1.2892275127
H,0,-4.436514627,0.2126804908,-1.7842032462
H,0,-5.0224117608,1.0831046395,0.7302759598

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.5674038
E (total electronic)+ZPVE = -1269.434476
Internal Thermal Energy = -1269.417039
Enthalpy = -1269.416095
Gibbs Free Energy = -1269.482524

C,0,-0.7567565887,-2.1342435741,-0.0154941964
C,0,-1.6317088931,-2.6459753825,-0.9789814299
C,0,0.2147837631,-2.8750520767,-0.6998993089
O,0,0.9939243715,-3.7332190598,-0.0070016576
O,0,-2.7636012316,-3.2716091898,-0.5886032789
H,0,-0.9408924199,-2.4115126149,1.0136081721
H,0,-1.5387619948,-2.3994150895,-2.0263515011
H,0,0.4968100747,-2.6653819847,-1.7208147296
H,0,1.5575770192,-4.2286184535,-0.6146316723
H,0,-3.2102488689,-3.6479271182,-1.3578363001
C,0,0.6812159581,1.5839038868,0.0703671902
F,0,-0.4849117016,2.2349459568,0.2256448358
C,0,0.5310030436,0.0662955669,0.3660375348
O,0,1.5348983045,-0.5470617069,0.6834852106
O,0,-0.6525939414,-0.3620729498,0.1902368832
F,0,1.5734921501,2.1268374273,0.9199611384
C,0,1.2045974181,1.8887684125,-1.3518439311
C,0,0.4068892242,1.2463858966,-2.5056115501
F,0,2.469980824,1.4555250145,-1.449105682
F,0,1.1908648898,3.21780986,-1.533885556
F,0,0.5226696263,-0.0764703271,-2.4536100676
F,0,0.8938850625,1.6684290064,-3.6641082701
F,0,-0.8754380897,1.5718814996,-2.4362088334

M06-2X/6-311+G(2d,p)
SMD, Solvent = Water

diOHCPr-Formate
E (total electronic) = -456.8728276
E (total electronic) + ZPVE = -456.766468
Internal Thermal Energy = -456.758198
Enthalpy = -456.757254
Gibbs Free Energy = -456.799672

C,0,-0.0564523367,-0.3504143015,-0.4601935984
C,0,-1.2308682897,-0.9131313304,0.2535664608
C,0,2.2394672442,-0.0610582401,-0.2288357901
O,0,2.1651830154,1.0784113142,-0.6057054764
O,0,1.2024858501,-0.8963215736,-0.1234495519
C,0,-0.7644065084,0.4953224732,0.5419278203
O,0,-1.4791776201,1.5774917585,0.019420889
O,0,-2.3762272638,-1.1111504685,-0.5241782116
H,0,-0.1789982234,-0.0866753813,-1.5035072539
H,0,-1.0386152703,-1.6502861714,1.0254256843
H,0,3.1641485328,-0.5619970848,0.0707045396
H,0,-0.2720444158,0.6549984412,1.4951595365
H,0,-2.3211156085,1.6402293002,0.4890519151
H,0,-3.1451911057,-0.8550457358,0.0018780367

TS–diOHCPr-Formate
E (total electronic) = -456.8228001
E (total electronic) + ZPVE = -456.719763
Internal Thermal Energy = -456.711317
Enthalpy = -456.710373
Gibbs Free Energy = -456.753606

C,0,-0.3829362916,-0.7447718255,-0.362235028
C,0,-1.5377232881,-1.3608617202,0.122742032
C,0,-0.7360790316,0.410514065,0.3369508307
O,0,-0.7280142088,1.5964418126,-0.295565641
O,0,-2.3586781794,-2.000134513,-0.7315068198
H,0,-0.295022286,-0.6526981739,-1.4380451746
H,0,-1.7389042759,-1.4710448224,1.1794129282
H,0,-0.8797083663,0.4202351899,1.4086844852
H,0,-1.0787937011,2.2815594937,0.2899902808
H,0,-3.1605937205,-2.2798693706,-0.2686896558
C,0,2.2289240682,-0.8281495326,-0.2799236681
O,0,2.2040307749,0.3021203923,-0.7667621928
O,0,1.2132732636,-1.5788368593,-0.0546830453
H,0,3.1920592426,-1.2809531361,0.0095026685

diOHCPr-Acetate
E (total electronic) = -496.1907855
E (total electronic) + ZPVE = -496.056736
Internal Thermal Energy = -496.046947
Enthalpy = -496.046003
Gibbs Free Energy = -496.091899

C,0,-1.0827010761,0.2240822382,0.8137140882
C,0,-1.7974501931,-0.5586160562,-0.2273273279
C,0,-0.4057995312,3.8073359081,1.0801699034
C,0,-0.1737113872,2.3402379601,1.2129424775
O,0,0.8074975117,1.8172087309,1.6844127268
O,0,-1.2170474676,1.6257782611,0.7425011834
C,0,-0.2880840737,-0.4796307656,-0.2326773139
O,0,0.4584792745,-1.5771420875,0.207629621
O,0,-2.4210808483,-1.7296579866,0.2162295745
H,0,-1.0513979753,-0.1879388525,1.8151026902
H,0,-2.3115563863,-0.0035017715,-1.0041360587
H,0,0.4695162662,4.3498151019,1.4245900422
H,0,-0.6182368815,4.0493979944,0.0386790361
H,0,-1.2773303127,4.0854943026,1.674211773
H,0,0.1605104371,0.129383351,-1.0100914789
H,0,0.3914287001,-2.2742941054,-0.4579285281
H,0,-2.2914270567,-2.4120202229,-0.4552254087

TS–diOHCPr-Acetate
E (total electronic) = -496.1378005
E (total electronic) + ZPVE = -496.006791
Internal Thermal Energy = -495.996957
Enthalpy = -495.996012
Gibbs Free Energy = -496.042441

C,0,-0.6996974837,-1.0175093119,-0.0583955099
C,0,-1.648432747,-1.5359633896,-0.9397653832
C,0,0.3233871096,-1.5825267356,-0.8200526803
O,0,1.2899981975,-2.2878713444,-0.2112780149
O,0,-2.7154269174,-2.1942392476,-0.4532521528
H,0,-0.7681538981,-1.3374832052,0.9742115334
H,0,-1.6385032542,-1.3227828448,-2.0000137843
H,0,0.4519209516,-1.3697693113,-1.8727103676
H,0,1.8689254574,-2.6923255217,-0.8719844597
H,0,-3.2274475053,-2.5740510605,-1.1803423969
C,0,0.2924202461,2.7250749375,1.1146393253
C,0,0.256777143,1.2274543691,0.9314952237
O,0,1.1512690714,0.5059199481,1.3892260888
O,0,-0.7519606026,0.7854480459,0.2580333915
H,0,1.0753483965,3.0072189691,1.8145093894
H,0,0.48649796,3.190518197,0.1464843153
H,0,-0.674671125,3.0821095059,1.4676404821

diOHCPr-2-Methylpropanoate
E (total electronic) = -574.8003468
E (total electronic) + ZPVE = -574.609583
Internal Thermal Energy = -574.596997
Enthalpy = -574.596053
Gibbs Free Energy = -574.649122

C,0,-1.1300250531,-0.0150081595,-0.5414020816
C,0,-2.2332395226,-0.8988178512,-0.084674814
C,0,2.4960671079,-0.4415349407,-0.1994926385
C,0,1.1764172792,0.2734020309,-0.3041893783
O,0,1.0010705811,1.459717935,-0.1596428523
O,0,0.1611283002,-0.5806690109,-0.5459004222
C,0,-1.7848150014,0.2672359441,0.7666727607

O,0,-2.5679184045,1.4249377744,0.8187049617
O,0,-3.4255751405,-0.8031781761,-0.8095484313
C,0,3.6565515034,0.5189670909,-0.4087984899
C,0,2.5606443215,-1.1130817908,1.1791314931
H,0,-1.3409062655,0.6684132227,-1.3550591367
H,0,-1.9650105919,-1.886735672,0.2732834914
H,0,2.5007101328,-1.2180009405,-0.9673870702
H,0,-1.2253747589,0.0215194023,1.6632905267
H,0,-3.3644144735,1.2289053105,1.329313969
H,0,-4.1610821492,-0.8808764947,-0.1883441572
H,0,3.6702812646,1.2822606411,0.3710142342
H,0,4.5972382662,-0.0308819165,-0.3644170969
H,0,3.5936919364,1.0168491632,-1.3772217544
H,0,1.7401496843,-1.8166473512,1.3220010284
H,0,3.5019858104,-1.6554886526,1.2724945572
H,0,2.519000173,-0.3597205584,1.9688423013

TS–diOHCPr-2-Methylpropanoate

E (total electronic) = -574.7470344
E (total electronic) + ZPVE = -574.559130
Internal Thermal Energy = -574.546690
Enthalpy = -574.545746
Gibbs Free Energy = -574.598923

C,0,-1.5216772691,-0.2777603723,-0.1900547093
C,0,-2.5368432524,-0.7022135673,0.6668536979
C,0,-1.8387716085,1.051418644,0.0906130651
O,0,-2.0003491483,1.9220698812,-0.9182435548
O,0,-3.4104943252,-1.6360112261,0.250985228
C,0,2.5095290054,-0.5566387981,0.1100455146
C,0,1.1080495478,-0.2156410199,-0.3798628182
O,0,0.9121041145,0.7104700438,-1.1756652761
O,0,0.1653419865,-0.9354987421,0.1293679222
C,0,3.5895551614,0.0081897381,-0.8002062462
C,0,2.6589925022,-0.0284079318,1.5409138734
H,0,-1.5950036923,-0.5857990778,-1.2258337707
H,0,-2.5811853058,-0.4099173306,1.7072507833
H,0,-1.8383440806,1.4494424807,1.0964796326
H,0,-2.3074848307,2.772636396,-0.5752223899
H,0,-4.1118848958,-1.7458235135,0.9075754588
H,0,2.5791326,-1.6469066574,0.1336291215
H,0,4.5738433199,-0.3041886712,-0.4464899806
H,0,3.4696104159,-0.3384156719,-1.8278258464
H,0,3.5618268788,1.0994421434,-0.8032190691
H,0,3.6525174765,-0.2659275207,1.9245794247
H,0,2.5389770413,1.0579135922,1.5584342954
H,0,1.9187023257,-0.4685858029,2.2097308653

diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.1062578
E (total electronic) + ZPVE = -613.887863
Internal Thermal Energy = -613.873964
Enthalpy = -613.873020
Gibbs Free Energy = -613.928744

C,0,-1.3059582948,0.1696643892,-0.7607680731
C,0,-2.4817136564,-0.4153260615,-0.0665034108
C,0,2.3052760918,-0.1001076984,-0.0950527857
C,0,0.9899740954,0.5206735611,-0.5216899991
O,0,0.8408042559,1.6439243277,-0.9410412984
O,0,-0.0436827682,-0.3337021604,-0.3900478587
C,0,-2.0655400144,1.012910731,0.2043305806
O,0,-2.7993109421,2.0627343936,-0.357356992
O,0,-3.5983949856,-0.6659043721,-0.8710632205
C,0,2.5691419334,-1.3360793577,-0.9651642388
C,0,3.4215722344,0.922139662,-0.2807952007
C,0,2.1998051181,-0.5086357455,1.3799987859
H,0,-1.4178455499,0.4095338434,-1.8113151971
H,0,-2.2893536147,-1.1299355318,0.7261741175
H,0,-1.605413946,1.2059559889,1.1675402683
H,0,-3.6446728026,2.1223938782,0.1062294634
H,0,-4.3898496906,-0.4305666764,-0.3697605235
H,0,3.5360056647,-1.7606094122,-0.6883363898
H,0,1.8034856714,-2.0979178756,-0.8177875272
H,0,2.6010889653,-1.0705108351,-2.0239438345
H,0,3.2511540039,1.8089687794,0.331671259
H,0,4.3698122597,0.4729590454,0.0187297445
H,0,3.5011384559,1.2335279863,-1.3235432776
H,0,3.1574848883,-0.9240263329,1.6993574793
H,0,1.9734071359,0.3541092249,2.0102803643
H,0,1.4289584914,-1.2648217514,1.5299937648

TS–diOHCPr-2,2-Dimethylpropanoate

E (total electronic) = -614.0529246
E (total electronic) + ZPVE = -613.837705
Internal Thermal Energy = -613.823752
Enthalpy = -613.822807
Gibbs Free Energy = -613.879804

C,0,-1.9085796963,-0.3752402274,-0.5883943176
C,0,-3.0031288155,-1.0079779929,0.0002977569
C,0,-2.3907936863,0.8652476216,-0.1711175424
O,0,-2.4500733766,1.8815918532,-1.0458064182
O,0,-3.6926889326,-1.9294706226,-0.6952394358
H,0,-1.7795927147,-0.5112301777,-1.6553586582
H,0,-3.2515328668,-0.8889238518,1.0461060823
H,0,-2.6027187399,1.088825219,0.8655512669
H,0,-2.8854550198,2.6424848628,-0.6376628047
H,0,-4.4730985288,-2.2032642769,-0.1941031145
C,0,2.1246420409,-0.6941618862,-0.0976674217
C,0,0.7237830703,-0.2347013197,-0.5252610612
O,0,0.5602367449,0.765796474,-1.2332297307
O,0,-0.2469857586,-0.9635994942,-0.0882175907
C,0,3.1920358595,0.2104776671,-0.7046531579
C,0,2.333517322,-2.1350833208,-0.5765802005
C,0,2.2068993886,-0.6381462459,1.4319464876
H,0,4.1798794265,-0.1333740197,-0.3902211056
H,0,3.1543672097,0.191580204,-1.7952474697
H,0,3.0703653464,1.2441581702,-0.3766436695
H,0,3.3386577893,-2.4667215109,-0.3063529383
H,0,1.6130179681,-2.8129740915,-0.1177552584
H,0,2.2317085207,-2.2043691477,-1.6624679883
H,0,3.2061091904,-0.9408438584,1.7535216191
H,0,2.025335527,0.3755585292,1.7976042015
H,0,1.4804687316,-1.3085905571,1.8926574697

diOHCPr-Fluoroacetate

E (total electronic) = -595.4251423
E (total electronic) + ZPVE = -595.298147
Internal Thermal Energy = -595.287623
Enthalpy = -595.286679
Gibbs Free Energy = -595.335119

C,0,0.2668921715,-0.9465698681,-0.2141181126
C,0,0.8757227413,-1.4790131591,1.0309376631
C,0,-0.8586498371,2.4244500936,-1.0321625322
C,0,-0.8469004892,0.9199468552,-1.0458511744
O,0,-1.6363548009,0.2272638687,-1.6304123043
O,0,0.1712315487,0.4596200836,-0.3114694936
C,0,-0.601672204,-1.6591695196,0.7648719278
O,0,-1.0797563827,-2.9070003168,0.354379882
O,0,1.7409607277,-2.5643689185,0.8616455966
F,0,-1.8786363365,2.8732660121,-1.8398729462
H,0,0.4912210246,-1.4560234649,-1.1431139618
H,0,1.1416804668,-0.7643467691,1.8018636029
H,0,-1.0234739275,2.7774016074,-0.0134825565
H,0,0.09202211,2.8033664457,-1.4075651854
H,0,-1.2751051713,-1.0551752104,1.3633499743
H,0,-1.0407876143,-3.5082828036,1.1097676605
H,0,1.5975439727,-3.1799119362,1.59225996

TS–diOHCPr-Fluoroacetate

E (total electronic) = -595.3769961
E (total electronic) + ZPVE = -595.252847
Internal Thermal Energy = -595.242392
Enthalpy = -595.241448
Gibbs Free Energy = -595.290253

C,0,-0.0784285339,-1.2896606572,-0.0437605572
C,0,-0.9981271323,-1.80972948,-0.956598883
C,0,0.9456246801,-1.8644791244,-0.7994436651
O,0,1.8852725765,-2.603688362,-0.1834082378
O,0,-2.0657505713,-2.4953396402,-0.5047733335
H,0,-0.1689171627,-1.6285512025,0.9813592035
H,0,-0.9762092631,-1.5650461689,-2.0097191637
H,0,1.1076736383,-1.6223151885,-1.8408500562
H,0,2.4666254051,-3.0096744108,-0.8409018516
H,0,-2.5518997962,-2.8724432548,-1.2507880852
C,0,0.905743941,2.4258059966,1.0866546179
C,0,0.8999804132,0.9170053615,0.9370596431
O,0,1.7986826856,0.2247357504,1.4067357971
O,0,-0.1204731898,0.4927221895,0.2790149897
F,0,2.0184936926,2.842151534,1.7969406942
H,0,0.9293927245,2.889560017,0.1004965254
H,0,0.0127218924,2.7447636403,1.6239973625

diOHCPr-Chloroacetate

E (total electronic) = -955.7866379
E (total electronic) + ZPVE = -955.661658
Internal Thermal Energy = -955.650631
Enthalpy = -955.649687
Gibbs Free Energy = -955.700132

C,0,-0.102916219,-1.0454759791,0.3593575489
C,0,-0.8342446083,-1.8151742162,-0.6785133912
C,0,0.5673247111,2.5231751124,0.5942670096
C,0,0.8283242557,1.0489533711,0.7602051687
O,0,1.8155067205,0.5410706552,1.2172968793
O,0,-0.2291239245,0.3606988216,0.3067779576
C,0,0.6762034229,-1.7384772547,-0.7039312981
O,0,1.4332095393,-2.8345799441,-0.2799038153
O,0,-1.4573464542,-2.9845534853,-0.2316101523
Cl,0,1.8910944269,3.5082770139,1.2530572513
H,0,-0.0596725134,-1.4638969819,1.3574380672
H,0,-1.3558868703,-1.2518349674,-1.4442769977
H,0,0.4610696852,2.7474974072,-0.4651311836
H,0,-0.3530156587,2.786681204,1.1098815219
H,0,1.1114546293,-1.1215309628,-1.4826436923
H,0,1.3926324287,-3.5135266402,-0.9659504658
H,0,-1.3743035711,-3.6530341536,-0.9240164082

TS–diOHCPr-Chloroacetate

E (total electronic) = -955.7385589
E (total electronic) + ZPVE = -955.616071
Internal Thermal Energy = -955.605297
Enthalpy = -955.604353
Gibbs Free Energy = -955.654520

C,0,-0.074754031,-1.3272733088,-0.1720136439
C,0,-0.9986003205,-1.8399235223,-1.0849729239
C,0,0.9465590462,-1.8995498738,-0.9333579989
O,0,1.8859544349,-2.6451773785,-0.3247487068
O,0,-2.0659735399,-2.525774668,-0.6333029182
H,0,-0.1633924205,-1.6713592063,0.8514930851
H,0,-0.9789546037,-1.589935836,-2.1369349062
H,0,1.1059553977,-1.6518957556,-1.973877561
H,0,2.4669709956,-3.0455217875,-0.9860655961
H,0,-2.5556140383,-2.8980977061,-1.3794572373
C,0,0.9104111967,2.3763111064,0.9677160642
C,0,0.9091159114,0.8606179025,0.8382162779
O,0,1.7796925077,0.1470342757,1.3216266799
O,0,-0.1067437039,0.4535646567,0.1583649831
Cl,0,2.2977143396,3.0108696016,1.9010478254
H,0,0.9467855465,2.8194343951,-0.024226267
H,0,0.0004302816,2.695338105,1.4694398436

diOHCPr-Bromoacetate

E (total electronic) = -3069.7538232
E (total electronic)+ZPVE = -3069.629274
Internal Thermal Energy = -3069.618188
Enthalpy = -3069.617244
Gibbs Free Energy = -3069.668280

C,0,-0.1574879068,-1.0864972225,0.3648311832
C,0,-0.8994809575,-1.8526465846,-0.6681832313
C,0,0.5192943651,2.4784270116,0.5835593482
C,0,0.7773770094,1.0061827684,0.7702710769
O,0,1.7587197313,0.4934623177,1.2317301598
O,0,-0.2845931238,0.3196347318,0.3177842189

C,0,0.610585026,-1.7742660463,-0.7098479851
O,0,1.3731771459,-2.8720414045,-0.3003347745
O,0,-1.5157514522,-3.0248531349,-0.2189970466
Br,0,1.9068690804,3.5813596576,1.3531030467
H,0,-0.1035185146,-1.5088823749,1.3607064747
H,0,-1.4307285418,-1.2872476916,-1.4258017387
H,0,0.4652933979,2.6947973432,-0.4812123647
H,0,-0.4258352876,2.74506753,1.0487610322
H,0,1.0364712563,-1.1530124495,-1.4903416067
H,0,1.3254607178,-3.5469816476,-0.9898806649
H,0,-1.437265946,-3.6915808039,-0.913642128

TS–diOHCPr-Bromoacetate

E (total electronic) = -3069.7053653
E (total electronic)+ZPVE = -3069.583552
Internal Thermal Energy = -3069.572563
Enthalpy = -3069.571618
Gibbs Free Energy = -3069.623107

C,0,-0.0717832702,-1.3616275198,-0.2125913867
C,0,-0.9973617384,-1.8530824016,-1.135134467
C,0,0.9511343874,-1.929185927,-0.9751785028
O,0,1.884670897,-2.6849104141,-0.3707994426
O,0,-2.0748819135,-2.5315372504,-0.6980620133
H,0,-0.166983474,-1.7163975976,0.8066919168
H,0,-0.9681897667,-1.5925168136,-2.1843284871
H,0,1.1149010499,-1.6727557085,-2.012943256
H,0,2.4682435183,-3.0790890789,-1.033622331
H,0,-2.5657235937,-2.8866502291,-1.4518409705
C,0,0.9040005436,2.3439058331,0.923761788
C,0,0.9213838668,0.8264232894,0.809964969
O,0,1.7928025085,0.1157172679,1.2916136824
O,0,-0.0994998377,0.4161547975,0.1351836089
Br,0,2.4080802933,3.1025880371,1.8939726104
H,0,0.9122178996,2.7780289191,-0.0720371792
H,0,0.0004696296,2.6549127965,1.4407604606

diOHCPr-Dichloroacetate

E (total electronic) = -1415.3766917
E (total electronic)+ZPVE = -1415.260676
Internal Thermal Energy = -1415.248863
Enthalpy = -1415.247919
Gibbs Free Energy = -1415.300762

C,0,1.6542675984,-0.2650830427,-0.5533639938
C,0,2.7148860519,0.7632428566,-0.4060383527
C,0,-1.9591768335,0.2364390762,-0.479558027
C,0,-0.6363145759,-0.4873058716,-0.2610019607
O,0,-0.5072692893,-1.5148028668,0.3401554585
O,0,0.3488322604,0.2177642804,-0.8096146715
C,0,2.2451942881,-0.0304555625,0.7928275586
O,0,3.0375612364,-1.0678398589,1.2910409402
O,0,3.9391415052,0.4523054619,-1.0041043717
Cl,0,-2.0450016065,1.533002214,0.7456604302
Cl,0,-3.3229109621,-0.871989476,-0.330877256
H,0,1.905442482,-1.1891249824,-1.0589376093
H,0,2.4080179217,1.8027847597,-0.4412837265
H,0,-1.9932773866,0.7038555492,-1.4576362851
H,0,1.6353481653,0.505295847,1.5132251387
H,0,3.7911056782,-0.677696193,1.7532257683
H,0,4.6455624664,0.7747598088,-0.4295680399

TS–diOHCPr-Dichloroacetate

E (total electronic) = -1415.3325518
E (total electronic)+ZPVE = -1415.219322
Internal Thermal Energy = -1415.207525
Enthalpy = -1415.206581
Gibbs Free Energy = -1415.260387

C,0,0.8195380927,-1.1070232352,-0.2270888494
C,0,1.7304039103,-1.3917311195,0.7944390931
C,0,-0.180736272,-1.5312009007,0.6540725276
O,0,-1.0737894581,-2.4531151618,0.24334179
O,0,2.8047254483,-2.1640837612,0.5305679829
H,0,0.9245274734,-1.6722162859,-1.1455515424
H,0,1.7056440815,-0.8844417774,1.7486783004
H,0,-0.3724687038,-1.0365553908,1.5965445874
H,0,-1.6456525024,-2.7047800267,0.9811634667
H,0,3.2898779876,-2.3374785726,1.3489421968
C,0,-0.4470408805,2.48001396,-1.2976269528
C,0,-0.3617722023,0.9457511941,-1.2356362847
O,0,-1.3474373066,0.2518387758,-1.426107131
O,0,0.8131101587,0.5501434096,-0.9132638423
Cl,0,-0.7758964077,3.0444114194,0.3698252494
Cl,0,-1.7098329354,3.0378986546,-2.407942487
H,0,0.4927675162,2.9209038184,-1.6071721049

diOHCPr-Trifluoroacetate

E (total electronic) = -793.9195649
E (total electronic) + ZPVE = -793.808972
Internal Thermal Energy = -793.797032
Enthalpy = -793.796087
Gibbs Free Energy = -793.849016

C,0,-0.7818190385,-0.2409266767,-0.4614785938
C,0,-1.9470130529,-0.7964292593,0.2697108414
C,0,2.8018478668,-0.642646963,0.1908239798
C,0,1.5028301069,0.0587124854,-0.2430786312
O,0,1.4798612383,1.1877355977,-0.6328056046
O,0,0.4864276719,-0.7722094765,-0.1144436515
C,0,-1.4878881373,0.6217242801,0.526173228
O,0,-2.2049465026,1.689931991,-0.017393981
O,0,-3.0878106489,-1.0238700116,-0.5038804192
F,0,3.8229852,0.1963089471,0.1238068477
F,0,3.0583670102,-1.6846669763,-0.597748498
F,0,2.7004998746,-1.0881877857,1.4412221471
H,0,-0.8975826476,-0.0062395699,-1.5120492297
H,0,-1.7433159611,-1.5131452122,1.057640005
H,0,-0.9921380912,0.8002065956,1.4744047568
H,0,-3.0345934788,1.7751315148,0.4704299611
H,0,-3.8603254099,-0.7669644806,0.0163838421

TS–diOHCPr-Trifluoroacetate

E (total electronic) = -793.8790004

E (total electronic) + ZPVE = -793.770792
Internal Thermal Energy = -793.759034
Enthalpy = -793.758090
Gibbs Free Energy = -793.810848

C,0,-1.0995460155,-0.5812814746,-0.4053100831
C,0,-2.2657714426,-1.1415272075,0.125435912
C,0,-1.4695374011,0.5805526601,0.2813674222
O,0,-1.5185566085,1.7505642697,-0.3885128527
O,0,-3.1433619153,-1.7487106078,-0.7023221864
H,0,-1.0466668537,-0.5041160502,-1.4851264051
H,0,-2.415684795,-1.2694272657,1.188191043
H,0,-1.5435593759,0.6206547091,1.3592693661
H,0,-1.8729093163,2.4407697706,0.1883238104
H,0,-3.9377136602,-1.9960935625,-0.2095593212
C,0,2.7909293159,-1.3058092459,0.1206498899
C,0,1.4607772031,-0.6198676952,-0.2721014043
O,0,1.4834336628,0.5323772039,-0.6638270998
O,0,0.4646360812,-1.400153328,-0.1199923777
F,0,3.0109203667,-2.3846552867,-0.6373437646
F,0,3.8288662468,-0.4887094885,-0.023743625
F,0,2.7620865077,-1.7105964009,1.3939296763

diOHCPr-Trichloroacetate

E (total electronic) = -1874.9601551
E (total electronic)+ZPVE = -1874.854875
Internal Thermal Energy = -1874.841732
Enthalpy = -1874.840787
Gibbs Free Energy = -1874.898048

C,0,-0.9329758902,-0.062587155,-0.7002770626
C,0,-2.0921355903,-0.6434932616,0.0211757951
C,0,2.6519098819,-0.4605276302,0.0082774183
C,0,1.3500225734,0.2206611947,-0.4765378957
O,0,1.3036697635,1.3582114441,-0.8369873282
O,0,0.3339001084,-0.6209552408,-0.3962922613
C,0,-1.6108610739,0.7537495464,0.3443059076
O,0,-2.3260617138,1.857582243,-0.125384616
O,0,-3.2495705416,-0.8123787879,-0.7428772555
Cl,0,4.0304627868,0.5991390638,-0.2735338992
Cl,0,2.8877597876,-1.9939284069,-0.8503231111
Cl,0,2.4706496714,-0.7604385438,1.7528416352
H,0,-1.0626274449,0.2276247405,-1.735174479
H,0,-1.8854800362,-1.4050667331,0.7650139825
H,0,-1.0927221358,0.8750816432,1.2901868057
H,0,-3.1465916902,1.9230652041,0.3805688269
H,0,-4.0088374562,-0.5791313206,-0.1927594626

TS–diOHCPr-Trichloroacetate

E (total electronic) = -1874.9193151
E (total electronic)+ZPVE = -1874.816687
Internal Thermal Energy = -1874.803611
Enthalpy = -1874.802667
Gibbs Free Energy = -1874.859696

C,0,-1.2818105825,-0.3991110003,-0.6610247571
C,0,-2.4303303053,-0.9781018406,-0.1123552556
C,0,-1.6061120215,0.7293230643,0.1007444789
O,0,-1.670550688,1.9336082295,-0.5035505903
O,0,-3.348602587,-1.5317498391,-0.9329256286
H,0,-1.2722912209,-0.2657414636,-1.7365366911
H,0,-2.5391147144,-1.160100376,0.9476396968
H,0,-1.6375932153,0.7123454595,1.1814107773
H,0,-2.0001812671,2.5936515759,0.1213075639
H,0,-4.1194304749,-1.8084794206,-0.4188280979
C,0,2.6073230088,-1.1133833119,-0.0666070051
C,0,1.2720115668,-0.4504857854,-0.5505577425
O,0,1.2799940112,0.7156490235,-0.8929338063
O,0,0.2798502678,-1.2456509893,-0.4768619515
Cl,0,4.0075193596,-0.1079477524,-0.4589197299
Cl,0,2.811409964,-2.7137128985,-0.8097046711
Cl,0,2.4853418986,-1.2881176749,1.7048224101

diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.5039977
E (total electronic)+ZPVE = -1269.367787
Internal Thermal Energy = -1269.350526
Enthalpy = -1269.349582
Gibbs Free Energy = -1269.414232

C,0,2.4847199183,-0.4943218293,0.1721669437
C,0,3.3235708096,-0.0723920002,-0.9754031205
C,0,2.8047858805,0.9516308736,0.0096601565
O,0,3.6674125061,1.485957027,0.9689934936
O,0,4.6619085781,-0.46865009,-0.916164457
C,0,-1.1139022567,-1.2137232891,0.3396249323
F,0,-1.0247740435,-2.3717772013,-0.3353044935
C,0,0.2815986353,-0.7653758673,0.8155070985
O,0,0.4593060717,-0.3212383186,1.9107097839
O,0,1.1718669177,-0.9340895608,-0.1405521958
F,0,-1.8979878242,-1.3976231284,1.4076487146
C,0,-1.8190285414,-0.2148198346,-0.6046443275
C,0,-1.9784751679,1.2124011932,-0.0506822979
F,0,-3.0399955633,-0.6938416839,-0.8712115092
F,0,-1.1236855195,-0.1357292238,-1.7460016957
F,0,-2.6531236244,1.2031937599,1.0878774276
F,0,-2.6306587921,1.9516741219,-0.9335692749
F,0,-0.7797463482,1.746272542,0.1578545378
H,0,2.9559556128,-1.0300010065,0.9862015141
H,0,2.8606743945,-0.068485086,-1.9560487007
H,0,2.0116039925,1.5993979305,-0.3482438704
H,0,4.2844017178,2.0798223464,0.5215798148
H,0,5.2054446463,0.2582873253,-1.2477184742

TS–diOHCPr-Heptafluorobutanoate

E (total electronic) = -1269.4645913
E (total electronic)+ZPVE = -1269.331455
Internal Thermal Energy = -1269.314045
Enthalpy = -1269.313101
Gibbs Free Energy = -1269.378984

C,0,-0.1804351748,2.6765316046,0.1653331707
F,0,-1.3565289174,3.2364427639,-0.1816442626

C,0,-0.3604259622,1.1665729016,0.4652596175
O,0,0.2214697557,0.6970129583,1.4251699124
O,0,-1.0904174675,0.581006275,-0.399293318
F,0,0.2799708818,3.3155970105,1.2519514357
C,0,0.7927276385,2.9694221361,-0.9948816732
C,0,2.1661521031,2.2878544013,-0.8761564784
F,0,0.9947226498,4.2936360082,-1.0572460043
F,0,0.2394134144,2.5649891837,-2.1460700864
F,0,2.7532086725,2.6070695903,0.2674935527
F,0,2.9383744849,2.675632261,-1.8800033204
F,0,2.0194115388,0.96813323,-0.9359418079
C,0,-0.9277028621,-1.1901735802,-0.3289558232
C,0,-1.2666629825,-1.9424365313,-1.4592439255
C,0,0.3228566672,-1.8125984531,-0.4340670471
O,0,0.8470068239,-2.4288272957,0.647219824
O,0,-2.3862765373,-2.6984311634,-1.4394619888
H,0,-1.4918300774,-1.3890079557,0.5745316622
H,0,-0.7765063443,-1.8066446306,-2.4131786597
H,0,0.9723012471,-1.6681158008,-1.2863521863
H,0,1.6637553908,-2.8827225886,0.3978103946
H,0,-2.4304189428,-3.2329063251,-2.244294988

V. Literature experimental data

Table S5. Solvolysis rate constants of dianisylmethyl carboxylates in aqueous ethanol mixtures at 25 °C and corresponding free energies of activation

Solvent [a]	Dianisylmethyl carboxylate	k / s^{-1}	log k	$\Delta G^{\ddagger}$ [b]	Ref.
90E10W	Heptafluorobutanoate	1.61×10^{1} [c]	1.21	15.81	2a
	Trifluoroacetate	1.06×10^{1} [c]	1.03	16.05	1a
	Trichloroacetate	5.70 [b]	0.76	16.42	1a
	Dichloroacetate	1.71×10^{-1} [c]	–0.77	18.50	1a
	Fluoroacetate	9.83×10^{-3}	–2.01	20.19	1a
	Chloroacetate	5.34×10^{-3}	–2.27	20.55	1a
	Bromoacetate	5.02×10^{-3}	–2.30	20.59	1a
	Formate	2.77×10^{-3}	–2.56	20.94	1a
	Acetate	4.41×10^{-5}	–4.36	23.40	2b
	2-Methylpropanoate (Isobutyrate)	1.36×10^{-5}	–4.87	24.09	1a
	2,2-Dimethylpropanoate (Pivalate)	4.73×10^{-6}	–5.33	24.72	1a
80E20W	Heptafluorobutanoate	3.84×10^{1} [c]	1.58	15.29	2a
	Trifluoroacetate	1.46×10^{1} [c]	1.16	15.86	2a
	Trichloroacetate	1.23×10^{1} [c]	1.09	15.97	1a
	Dichloroacetate	2.90×10^{-1} [c]	–0.54	18.19	1a
	Fluoroacetate	1.93×10^{-2}	–1.71	19.79	1a
	Chloroacetate	1.06×10^{-2}	–1.97	20.15	1a
	Bromoacetate	1.07×10^{-2}	–1.97	20.14	1a
	Formate	6.11×10^{-3}	–2.21	20.47	1a
	Acetate	9.06×10^{-5}	–4.04	22.97	2b
	2-Methylpropanoate (Isobutyrate)	2.73×10^{-5}	–4.56	23.68	1a
	2,2-Dimethylpropanoate (Pivalate)	9.48×10^{-6}	–5.02	24.31	1a
70E30W	Heptafluorobutanoate	5.15×10^{1} [c]	1.71	15.12	2a
	Trifluoroacetate	3.45×10^{1} [c]	1.54	15.36	2a
	Trichloroacetate	1.99×10^{1} [c]	1.30	15.68	1a
	Dichloroacetate	4.65×10^{-1} [c]	–0.33	17.91	1a
	Fluoroacetate	3.05×10^{-2}	–1.52	19.52	1a
	Chloroacetate	1.63×10^{-2}	–1.79	19.89	1a
	Bromoacetate	1.65×10^{-2}	–1.78	19.89	1a
	Formate	1.10×10^{-2}	–1.96	20.13	1a
	Acetate	1.50×10^{-4}	–3.82	22.67	2b
	2-Methylpropanoate (Isobutyrate)	3.32×10^{-5}	–4.48	23.56	1a

Solvent [a]	Dianisylmethyl carboxylate	k / s^{-1}	log k	$\Delta G^{\ddagger}$ [b]	Ref.
	2,2-Dimethylpropanoate (Pivalate)	1.35×10^{-5}	–4.87	24.10	1a
60E40W	Heptafluorobutanoate	9.51×10^{1} [c]	1.98	14.75	2a
	Trifluoroacetate	5.37×10^{1} [c]	1.73	15.09	2a
	Trichloroacetate	3.01×10^{1} [c]	1.48	15.44	1a
	Dichloroacetate	6.25×10^{-1} [c]	–0.20	17.73	1a
	Fluoroacetate	4.80×10^{-2}	–1.32	19.25	1a
	Chloroacetate	2.47×10^{-2}	–1.61	19.65	1a
	Bromoacetate	2.51×10^{-2}	–1.60	19.64	1a
	Formate	1.75×10^{-2}	–1.76	19.85	1a
	Acetate	2.34×10^{-4}	–3.63	22.41	2b
	2-Methylpropanoate (Isobutyrate)	4.58×10^{-5}	–4.34	23.37	1a
	2,2-Dimethylpropanoate (Pivalate)	2.09×10^{-5}	–4.68	23.84	1a

[a] Binary solvents are v/v at 25 °C. E = ethanol, W = water. [b] in kcal mol^{-1} [c] Calculated by using equation $\log k = s_f (E_f + N_f)$. $E_f = 0.00$ for the dianisylmethyl electrofuge.

Table S6. pK_a values of carboxylic acids and corresponding free energies of dissociation

Carboxylic acid	$\Delta G°$ (kcal/mol)	pK_a	Ref.
Formic	5.12	3.75	3a
Acetic	6.49	4.76	3a
Propanoic	6.64	4.87	3a
Butanoic	6.59	4.83	3a
2-Methylpropanoic	6.60	4.84	3a
2,2-Dimethylpropanoic	6.86	5.03	3a
Phenylacetic	5.88	4.31	3a
Fluoroacetic	3.53	2.59	3a
Chloroacetic	3.92	2.87	3a
Bromoacetic	3.96	2.90	3a
Difluoroacetic	1.69	1.24	3b
Dichloroacetic	1.84	1.35	3a
Dibromoacetic	2.02	1.48	3b
Trifluoroacetic	0.31	0.23	3b
Trichloroacetic	0.90	0.66	3a
Tribromoacetic	0.90	0.66	3b
Heptafluorobutanoic	0.14	0.10	3c

Carboxylic acid	**$\Delta G°$ (kcal/mol)**	**pK_a**	**Ref.**
3,3,3-Trifluoropropanoic	4.19	3.07	3b
Pentafluoropropanoic	0.25	0.18	3e
Cyanoacetic	3.37	2.47	3a
Nitroacetic	2.02	1.48	3a
Propenoic	5.80	4.25	3a
Propynoic	2.51	1.84	3a
2-Oxopropanoic	3.26	2.39	3a
2-Oxobutanoic	3.41	2.50	3a
3-Oxobutanoic	4.94	3.62	3d
2-Hydroxyethanoic	5.22	3.83	3a
2-Hydroxypropanoic	5.14	3.77	3d
2,3-Dihydroxypropanoic	4.80	3.52	3a
Malonic, 1.ionization	3.89	2.85	3a
Malonic, 2.ionization	7.78	5.70	3a
Oxalic, 1. ionization	1.71	1.25	3d
Oxalic, 2. ionization	5.80	4.25	3d

VI. References

1. (a) M. Matić, B. Denegri, O. Kronja, *Eur. J. Org. Chem.* **2014**, 1477–1486.
   (b) N. Streidl, B. Denegri, O. Kronja, H. Mayr, *Acc. Chem. Res.*, 2010, **43**, 1537−1549.
2. (a) B. Denegri, O. Kronja, *J. Org. Chem.* **2009**, *74*, 5927–5933.
   (b) B. Denegri, O. Kronja, *Croat. Chem. Acta* **2010**, *83*, 223–226.
3. (a) CRC *Handbook of Chemistry and Physics*, 87th ed.; CRC Press; **2006-2007**.
   (b) W. P. Jencks, J. Regenstein, *Ionization Constants of Acids and Bases* in *Handbook of Biochemistry and Molecular Biology*, G. D. Fasman, ed.; CRC Press, Cleveland. **1976**, p. 305-351.
   (c) R. J. P. Cannell, *Natural Products Isolation*, Humana Press Inc., New Jersey, **1998**, p. 180.
   (d) R. M. C. Dawson, *Data for Biochemical Research*, 3rd. ed.; Oxford University Press, New York, **1986**.
   (e) Chemicalbook, http://www.chemicalbook.com/