Electronic Supplementary Information for

Green Solvents from Glycerol. Synthesis and Physico-Chemical properties of Alkyl Glycerol Ethers.

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Table 1S. Physico-chemical properties of glycerol-based solvents.

Solvents	E_T^N	π^*	α	μ (D)	ε	Kirkwood function[a]	ΔlogP98	b.p (°C)	AHvap (kJ/mol)	Kinematic viscosity (cSt)	Dynamic viscosity (cP)	density (g/cm3)	n_D^{20}	Dielectric function[b]
1,0,0	0,71	0,86	0,83	3,416	21,878	0,4664	-0,9996	222	43,03	34,011	37,719	1,109	1,4220	0,2026
2,0,0	0,69	0,77	0,86	3,424	18,623	0,4608	-0,6508	221	45,02	33,251	35,139	1,0568	1,4394	0,2084
4,0,0	0,68	0,68	0,91	3,148	12,553	0,4425	0,3291	249	41,11	42,126	42,030	0,99772	1,4418	0,2092
1,0,1	0,61	0,73	0,72	2,929	12,963	0,4443	-0,5911	170	30,99	3,430	3,416	1,0092	1,4155	0,2004
3i,0,1	0,49	0,71	0,47	2,508	7,861	0,4103	0,1352	188	38,21	3,567	3,376	0,94635	1,4176	0,2011
4,0,1	0,48	0,96	0,27	2,424	6,945	0,3993	0,7376	208	58,34			0,93815	1,4242	0,2034
4i,0,1	0,49	0,62	0,55	2,353	6,561	0,3938	0,6007	200	50,92			0,93029	1,4208	0,2022
4t,0,1	0,44	0,71	0,36	2,359	6,612	0,3945	0,3402	195	55,71			0,93419	1,4212	0,2024
3i,0,4	0,43	0,16	0,77				1,4639	223	56,93	5,053	4,590			
4,0,4	0,45	1,09	0,10	2,393	5,642	0,3779	2,0663	248	68,36	6,061	5,525	0,91169	1,4271	0,2043
4t,0,4	0,39	0,75	0,22	2,259	5,163	0,3676	1,6689	230	44,50			0,9024	1,4257	0,2039
4i,0,4	0,46	0,57	0,50	2,257	5,149	0,3672	1,9294	229	55,69			0,90057	1,4258	0,2039
3i,0,2	0,45	0,75	0,36	2,541	7,386	0,4049	0,4840	187	26,18			0,93378	1,4176	0,2011
4,0,2	0,45	0,96	0,21	2,459	6,599	0,3944	1,0864	220	44,01			0,92774	1,4237	0,2032
4t,0,2	0,41	0,62	0,36	2,317	5,965	0,3840	0,6890	204	43,68			0,9172	1,4214	0,2024
4i,0,2	0,46	0,71	0,40	2,33	5,997	0,3846	0,9495	214	40,86			0,91337	1,4214	0,2024
3i,0,3i	0,46						0,8615	202	40,68					
4,0,3i	0,50	1,25	0,08	2,314	5,614	0,3773	1,4639	224	53,32			0,90826	1,4238	0,2032
4t,0,3i	0,37	0,62	0,29				1,0665	202	46,09					
4i,0,3i	0,44	0,57	0,47				1,3270	215	47,21					
3i,0,3F	0,59	0,71		3,361	11,986	0,4399	1,1426	176	37,03	5,087	6,895	1,35556	1,3821	0,1888
4,0,3F	0,60	0,84	0,70	3,446	10,235	0,4301	1,7450	210	57,40			1,11406	1,3903	0,1917
4t,0,3F	0,57	0,53	0,61	3,642	11,197	0,4359	1,3476	199	45,79	7,748	8,609	1,1112	1,3868	0,1905
4i,0,3F	0,60	0,57	0,79	3,431	10,013	0,4287	1,6081	205	56,77			1,09854	1,3890	0,1913
3F,0,3F	0,70	0,38	0,82	4,098	14,616	0,4504	1,4237	197	51,00	5,883	8,140	1,38367	1,3522	0,1779
5F,0,5F	0,70	0,56	1,04	3,941	10,438	0,4314	2,4069	204	43,92			1,4727	1,3354	0,1715
7F,0,5F	0,69	0,55	1,01	3,903	8,629	0,4178	3,3901	206	57,57	12,554	19,596	1,5609	1,3298	0,1694
1,1,1				2,219	6,838	0,3978	-0,1826	150	30,24			0,94275	1,4032	0,1962
3i,1,1				1,993	4,918	0,3616	0,5437	170	39,88	1,144	1,025	0,89565	1,4044	0,1966
3i,4,1	0,15	-0,06	0,32				1,8724	215	45,89					
4t,1,1	0,21	0,53	0,02				0,7487	180	34,63					
4t,4,1							2,0774	219	46,77					
4,1,1	0,18						1,1461	199	51,82					
4,4,1							2,4748	234	59,08					
4i,1,1							1,0092	193	51,20					
4i,4,1							2,3379	227	50,63					
3i,2,1	0,17	-0,02	0,35				0,8925	161	26,02					
3i,1,2	0,17	0,15	0,22				0,8925	183	48,72					
4t,2,1							1,0975	190	43,99					
4t,1,2	0,15	-0,23	0,47				1,0975	193	43,18					
4,2,1	0,16	0,10	0,23				1,4949	209	51,60					
4,1,2	0,16	0,16	0,21				1,4949	209	52,78					
4i,2,1							1,3580	198	45,99					
4i,1,2	0,16	0,32	0,07				1,3580	201	51,59					
3i,2,2							1,2413	192	43,90					

4t,2,2	0,16	-0,17	0,44				1,4463	199	37,39					
4,2,2	0,16	0,15	0,21				1,8437	217	49,93					
4i,2,2		0,41					1,7068	210	54,18					
3i,1,4	0,16	0,31	0,07	2,175	4,8	0,3585	1,8724	218	61,87	1,865	1,669	0,89516	1,4135	0,1998
3i,2,4							2,2212	222	51,57					
4t,1,4	0,14	0,42	-0,04				2,0774	234	63,06					
4t,2,4							2,4262	211	60,04					
4,1,4	0,15	0,24	0,10	2,184	4,68	0,3552	2,4748	244	48,78	4,316	3,783	0,87652	1,4191	0,2017
4i,1,4	0,15	0,39	0,00				2,3379	226	51,86					
4i,2,4							2,6867	241	63,32					
4,4,4		1,12		2,39	4,7	0,3558	3,8035	270	77,06	3,151	2,721	0,86358	1,4237	0,2032
3i,1,3F		0,88		3,506	9,938	0,4281	1,5511	180	39,23			1,0672	1,3748	0,1862
4t,1,3F	0,37	0,69	0,24	3,484	9,266	0,4232	1,7561	185	47,19	2,046	2,139	1,0456	1,3816	0,1886
4,1,3F							2,1535	207	42,23					
3F,1,3F	0,55	1,04	0,36	4,235	13,744	0,4473	1,8322	178	45,23	1,810	2,330	1,2871	1,3476	0,1762
3F,2,3F	0,60	0,91	0,55	4,268	12,81	0,4437	2,1810	171	50,08			1,2266	1,3516	0,1777
3F,4,3F	0,57	1,09	0,36				3,1609	208	52,77					

[a] $(\varepsilon-1)/(2\varepsilon+1)$ [b] $(n^2-1)/(2n^2+1)$

Comment on π^* and α values: π^* values display a somewhat erratic behaviour. In general, they are higher for alcohols (diethers) than for triethers, and also higher for those compounds bearing fluoroalkyl substituents, but there are some exceptions, and in particular some compounds have negative values, normally associated to a very low polarity (as is the case of perfluoroalkanes). Obviously, these values are not reasonable, and point to the difficult measurement of π^* for these systems. In fact, in some cases it was impossible even to have an estimation of π^*, since the UV spectrum of p-NO_2-anisole showed a complex structure, with several superimposed bands, which is totally unusual. Obviously, as α values were estimated from $E_T(30)$ and π^*, they are also affected for α the errors in π^* determinations, with some values unusually high in those cases where the π^* values are negative. Otherwise, the α values are in line with the observations made for $E_T(30)$, and cover a wide range of hydrogen-bond donor abilities, from weak to very strong.

List of solvent names abbreviations used in Figures 1, 4, 5, 6, 7

Ace: Acetone
ACN: Acetonitrile
BuOH: *n*-Butanol
DCM: Dichloromethane
DE: Diethylether
DMF: Dimethylformamide
DMSO: Dimethylsulfoxide
EA: Ethyl acetate
EC: Diethyl carbonate
EG: Ethylene glycol
Fur: Furan
Gly: Glycerol
Hx: *n*-Hexane
HxOH: *n*-Hexanol
MeOH: Methanol
NM: Nitromethane
Naph: Naphtalene
OcOH: *n*-Octanol
PCB: Pentachlorobenzene
PhOH: Phenol
PrOH: *n*-Propanol
p-Xyl: *p*-Xylene
TAC: Triacetin
TFE: 2,2,2-Trifluoroethanol
THF: tetrahydrofuran
Tol: Toluene
W: Water

Table 2S. Experimental vapour pressures P* (mm Hg) of some representative glycerol-based solvents at different temperatures.

T (K)	Solvent						
	1,0,4t	1,1,4t	4,0,4	4,0,4t	3i,0,3i	3F,0,3F	3F,1,3F
293.15	0.275	0.510	0.018	0.060	0.311	0.270	0.285
298.15	0.420	0.751	0.030	0.105	0.480	0.400	0.429
303.15	0.620	1.084	0.055	0.176	0.700	0.571	0.640
313.15	1.260	2.175	0.138	0.442	1.399	1.130	1.359
323.15	2.495	4.121	0.335	0.885	2.721	2.030	2.710
333.15	4.549	7.546	0.680	1.811	4.879	3.611	5.238
343.15	8.061	13.09	1.320	3.869	8.273	6.153	9.944
353.15	13.71	22.46	2.479	6.560	13.98	10.24	17.43
363.15	22.49	37.75	4.678	11.11	23.24	16.78	29.28
373.15	35.80	60.52	8.199	19.24	36.09	26.76	50.96

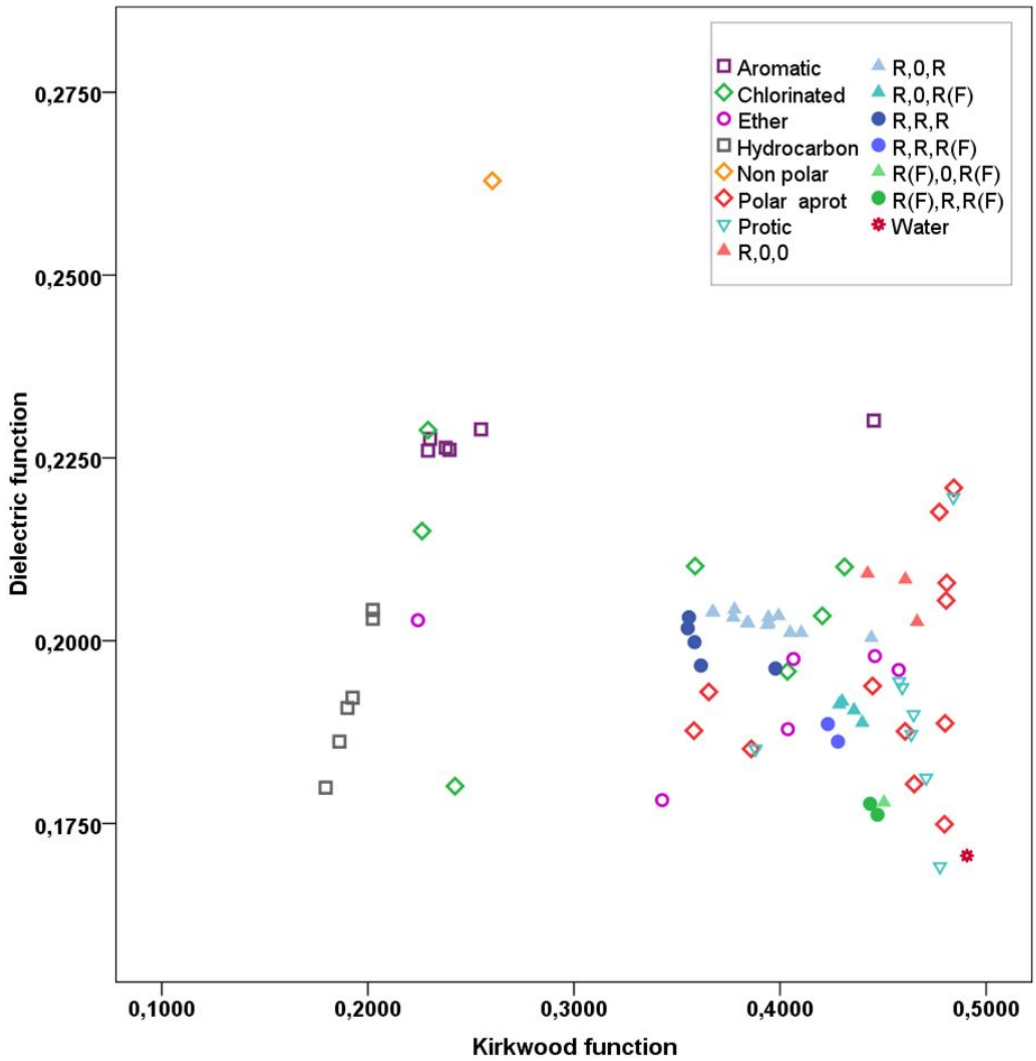

Figure 1S. Kirkwood function *vs*. Dielectric function plot for a series of common organic solvents and glycerol-derived solvents.

Experimental procedures for the physico-chemical properties measurements

Solvatochromic parameters

A double beam photometer model Unicam UV-4 was used to determine the spectroscopic parameters.
The scan speed was 30 nm·min^{-1}, with a resolution of 0,1 nm. The cell path was 1 cm, and their volume was 1,5 mL. Concentration of dyes was between $1\cdot10^{-2}$ and $4\cdot10^{-2}$ mg·mL^{-1} for Dimroth dye's ($E_T(30)$ determination) and between $2\cdot10^{-1}$ and $6\cdot10^{-1}$ mg·mL^{-1} for p-nitroanisole (π^* determination). Sometimes it was necessary to use sonication to improve the solution process.
Spectra were registered between 400 and 800 nm for $E_T(30)$ parameter and between 200 and 400 nm for π^*.

$$E_T(30)(kcal\cdot mol^{-1}) = h\cdot c\cdot \bar{\nu}\cdot N_A = 2{,}859\cdot 10^{-3}\cdot \bar{\nu}(cm^{-1})$$

$$E_T^N = \frac{E_T(30) - 30{,}7}{32{,}4}$$

$$\pi^* = \frac{(\bar{\nu}\cdot 10^{-3}\cdot cm^{-1}) - 34{,}17}{-2{,}410}$$

Dielectric permittivity and dipole moment.

Dielectric permittivity data were obtained with a WTW (DM01) dipolmeter (Kahlsico) which works at 2 MHz by a beat heterodyne method. The sample holding cells are provided with a water jacket for maintaining the constant temperature of the liquid being measured. The uncertainty is estimated in $\pm$0,001.
The average dipole moment $\langle\mu^2\rangle^{1/2}$ was calculated from measured dielectric permittivities, refraction indices and densities through the Onsager's equation:[1S]

$$\mu^2 = \frac{9kTM}{4\pi N_A \rho}\frac{(\varepsilon - n^2)(2\varepsilon + n^2)}{\varepsilon(n^2+2)^2}$$

where

k = Boltzman's constant
T = temperature in ºK
M = molar mass
N_A = Avogadro's number
ρ = density
n = refractive index
ε = dielectric permittivity

Refraction index.

Refractive index was determined using a Zeiss refractometer with temperature controlled exchangeable prisms and a sodium lamp as light source. The uncertainty is estimated in ±0.00002.

Hydrophobicity and water content.

Hydrophobicity, measured as logP values, was estimated using the Ghose and Crippen atom contribution method through the ΔLogP98 refinement.[2S]
To determine water content in solvents under storage conditions, solvents were kept in closed bottles under air atmosphere during 6 months. The determination of water in solvents under saturated conditions was carried out after washing those solvents with water during 30 min.
To determine the quantity of water in solvents, a Karl–Fisher closed volumetric system was used. First of all exact concentration of Karl–Fisher reagent (Iodine–sulfur dioxide–pyridine, from Fluka) was determined, using $Zn(AcO)_2\cdot 2H_2O$ (16,42 % of water) (200 mg) dissolved in 20 mL of dry methanol (Hydranal®, from Fluka), the result was 5,254 mg H_2O/mL reagent. After that three blank measures were done to determine the quantity of water in methanol dry (Hydranal®), the result was 171 mg/L. To determine the quantity of water in glycerol-based solvents, certain quantity of solvent (5 g) was dissolved in 20 mL of dry methanol (Hydranal®), and then was titrated with Karl-Fisher reagent.

Viscosities.

Ubbelohde viscometers (Schott) of relatively long flow times (100 s to 600 s) were used to minimize the kinetic energy corrections. At least three readings of the flow time with variations not exceeding ±0,1 s were taken for each liquid. The viscosities were calculated from the average flow time, t, by means of the equation

$$\nu = At - \left(\frac{B}{t}\right)$$

where ν is the kinematic viscosity. A and B are the viscometers constants that were determined by using values from literature.[3S] The viscometer was held in a water bath whose temperature was controlled to within ±10 mK. Three different viscometers were used during the course of this investigation. The uncertainty in the kinematic viscosity measurements is not worse than $\pm 2 \times 10^{-9}$ $m^2.s^{-1}$.
Dynamic viscosity was calculated according to the equation

$$\eta = \nu\rho$$

where ν and ρ are the kinematic viscosity and the density, respectively.

Densities.

A densimeter (Anton Paar DMA 60/DMA 602) was used for density measurements. The densimeter operates at 298.15 K and sample density is calculated from the vibration period with un uncertainty of ±0.00002 $g.cm^{-3}$.

Boiling point.

Differential scanning calorimetry (DSC) was carried out using Indium as reference (m.p = 156,61 ºC and ΔH_f = 28,71 $J \cdot g^{-1}$) in a DSC-MDSC TA Instruments 2910. It was used samples between 1 and 2 mg in aluminium perforated capsules with a heating rate of 20ºC·min^{-1}. Boiling point temperatures were assigned at offset point of the scanning. The standard error of the method was estimated in 1.6 ºC, based on measurements made on glycerol and three glycerol derivatives, covering a range of 188–290 ºC in b.p.

Vapour pressures.

The vapour pressure measurements were performed by a static method. The apparatus is similar to that of Marsh[4S] except for some experimental details, the most important is the replacement of the mercury manometer by electronic gauges.
Each liquid were degassed by magnetic stirring under its own vapour pressure and the vapour + air pumped away periodically. A glass cell with PTFE junction, filled with around 10–12 cm^3 of liquid degassed was connected to the manometer system, previously evacuated, and then the liquid sample was introduced by gravity into the vapour- pressure cell which was joined to a stainless steel pipe. The pressure was measured with a set of three Barocell 659 capacitance manometers (Edwards absolute models) each one with a different pressure range (0–10 torr, 0–100 torr, 0–1000 torr). To prevent condensation effects the temperature of the manometers was maintained at 396.15 ºK. The temperature of the liquid sample was measured by means of a digital Pt 100 thermometer with an uncertainty within ±1 mK. Manometer lectures were read with a resolution of 0.005% of full scale.

References

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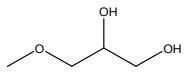
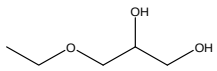
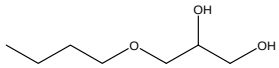
3S. *TRC–Thermodynamic Tables–Non Hydrocarbons;* Thermodynamic Research Center, The Texas A&M University System: College Station, TX, 1971; p. 5030.
4S. K. N. Marsh, *Trans. Faraday Soc.*, 1968, *64*, 883.

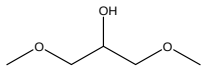
Table 3S. Full characterization of the glycerol-derived solvents prepared

^{1}H-RMN (CDCl3, δ ppm, 400 MHz); ^{13}C-RMN (CDCl3, δ ppm, 400 MHz); FT-IR (cm^{-1}); Elemental analysis (%); μ (D); b. p. (ºC); ΔH_{vap}^{eb} (kJ·mol^{-1}); P_{vap}^{298} (mm Hg); H_2O^{sol} (mg·g^{-1}); ν^{20} (cSt); η^{20} (cP); ρ^{20} (g·cm^{-3})

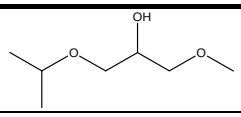
Name	3-methoxy-1,2-propanediol					**Structure**					
Code	1,0,0										
CAS	623-39-2										
^{1}H-RMN	3.294 (s, 3H); 3.338, 3.334 (d, 1H); 3.353, 3.356 (d, 1H); 3.451, 3.467, 3.480,3.496 (dd, 1H); 3.551, 3.561, 3.580, 3.589 (dd, 1H); 3.750-3.802 (m, 1H); 3.912 (sa, 1H);4.088 (sa, 1H)										
^{13}C-RMN	58.931; 63.680; 70.587; 73.851										
FT-IR	1111; 1160; 2868; 2923; 2966; 3399										
m/z	106.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
45.27	9.50	45.23	0.00			45.1	9.6				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.71	**μ**	3.416	**b. p.**	222	n_D^{20}	1.4220	**log P**	-0.9996	ν^{20}	34.011
π*	0.86	**ε**	21.878	ΔH_{vap}^{eb}	43.03	$f_{(dielectric)}$	0.2026	H_2O^{sol}	Miscible	η^{20}	37.719
α	0.83	$f_{(kirkwood)}$	0.4664	P_{vap}^{298}	n.a.					ρ^{20}	1.1090

Name	3-ethoxy-1,2-propanediol					**Structure**					
Code	2,0,0										
CAS	1874-62-0										
^{1}H-RMN	1.096, 1.114, 1.131 (t, 3H); 3.366, 3.375, 3.381, 3.87 (dd, 2H); 3.415, 3.433, 3.450, 3.468 (c, 2H); 3.485, 3.500, 3.565, 3.593 (dd, 2H); 3.773 (m, 1H); 3.871 (sa, 1H); 4.031 (sa, 1H)										
^{13}C-RMN	14.799; 63.773; 66.674; 70.660; 71.691										
FT-IR	1114; 1174; 2874; 2932; 2976; 3390										
m/z	120.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
49.98	10.07	39.95	0.00			49.2	10.5				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.69	**μ**	3.424	**b. p.**	221	n_D^{20}	1.4394	**log P**	-0.6508	ν^{20}	33.251
π*	0.77	**ε**	18.623	ΔH_{vap}^{eb}	45.02	$f_{(dielectric)}$	0.2084	H_2O^{sol}	Miscible	η^{20}	35.139
α	0.86	$f_{(kirkwood)}$	0.4608	P_{vap}^{298}	n.a.					ρ^{20}	1.0568

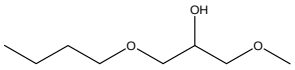
Name	3-*n*-butoxy-1,2-propanediol					**Structure**					
Code	4,0,0										
CAS	624-52-2										
^{1}H-RMN	0.854, 0.872, 0.890 (t, 3H); 1.328 (m, 2H); 1.449, 1.469, 1.486, 1.502, 1.523 (q, 2H); 2.841 (sa, 1H); 3.430 (m, 1H) 3.553 (m, 2H); 4.775 (sa, 1H); 4.821 (sa, 1H)										
^{13}C-RMN	13.730; 18.795; 34.684; 62.288; 63.977; 70.585; 71.351										
FT-IR	1120; 1186; 2873; 2941; 2974; 3410										
m/z	148.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
56.73	10.88	32.39	0.00			56.9	10.5				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.68	**μ**	3.148	**b. p.**	249	n_D^{20}	1.4418	**log P**	0.3291	ν^{20}	42.126
π*	0.68	**ε**	12.553	ΔH_{vap}^{eb}	41.11	$f_{(dielectric)}$	0.2092	H_2O^{sol}	Miscible	η^{20}	42.030
α	0.91	$f_{(kirkwood)}$	0.4425	P_{vap}^{298}	n.a.					ρ^{20}	0.9977

Name	1,3-dimethoxy-2-propanol	**Structure**	
Code	1,0,1		
CAS	623-69-8		
^{1}H-RMN	2.783 (sa, 1H); 3.344 (s, 6H); 3.362, 3.371, 3.487, 3.497, 3.408, 3.422, 3.433 (ddd, 4H); 3.879-3943 (m, 1H)		
^{13}C-RMN	59.078; 69.132; 73.747		

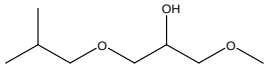
FT-IR	1191; 2870; 2929; 2969; 3440										
m/z	120.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**	**H**		**O**	**F**	
49.98	10.07		39.95	0.00		50.1	9.9				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.61	**μ**	2.929	**b. p.**	170	n_D^{20}	1.4155	**log P**	-0.5911	ν^{20}	3.430
π*	0.73	**ε**	12.963	ΔH_{vap}^{eb}	30.99	$f_{(dielectric)}$	0.2004	H_2O^{sol}	Miscible	η^{20}	3.416
α	0.72	$f_{(kirkwood)}$	0.4443	P_{vap}^{298}	n.a.					ρ^{20}	1.0092

Name	1-*iso*-propoxy-3-methoxy-2-propanol	**Structure**	
Code	3i,0,1		
CAS	53146-34-2		
^{1}H-RMN	1.131, 1.147 (d, 6H); 2.623 (sa, 1H); 3.362 (s, 3H); 3.385-3.487 (m, 4H); 3.547, 3.562, 3.578, 3.593, 3.608 (q, 1H); 3.889 (m, 1H)		
^{13}C-RMN	21.776; 58.897; 69.068; 69.250; 71.923; 73.817		
FT-IR	1075; 1126; 2874; 2923; 2971; 3460		
m/z	148.0		

Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**	**H**		**O**	**F**	
56.73	10.88		32.39	0.00		56.5	10.9				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.49	**μ**	2.508	**b. p.**	188	n_D^{20}	1.4176	**log P**	0.1352	ν^{20}	3.567
π*	0.71	**ε**	7.861	ΔH_{vap}^{eb}	38.21	$f_{(dielectric)}$	0.2011	H_2O^{sol}	Miscible	η^{20}	3.376
α	0.47	$f_{(kirkwood)}$	0.4103	P_{vap}^{298}	n.a.					ρ^{20}	0.9464

Name	1-*n*-butoxy-3-methoxy-2-propanol	**Structure**	
Code	4,0,1		
CAS	13021-51-7		
^{1}H-RMN	0.854, 0.873, 0.891 (t, 3H); 1.274, 1.292, 1.310, 1.329, 1.348, 1.367 (m, 2H); 1.483, 1.499, 1.519, 1.536, 1.553 (q, 2H); 2.745 (sa, 1H); 3.341 (s, 3H); 3.364-3,455 (m, 6H); 3.878, 3.891, 3.904, 3.916, 3.931 (q, 1H)		
^{13}C-RMN	13.646; 19.011; 31.410; 58.883; 69.061; 71.077; 71.672; 73.798		
FT-IR	1114; 1460; 2870; 2930; 2957; 3437		
m/z	162.0		

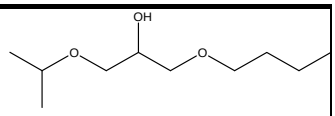
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**	**H**		**O**	**F**	
59.23	11.18		29.59	0.00		59.1	11.5				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.48	**μ**	2.424	**b. p.**	208	n_D^{20}	1.4242	**log P**	0.7376	ν^{20}	n.a.
π*	0.96	**ε**	6.945	ΔH_{vap}^{eb}	58.34	$f_{(dielectric)}$	0.2034	H_2O^{sol}	Miscible	η^{20}	n.a.
α	0.27	$f_{(kirkwood)}$	0.3993	P_{vap}^{298}	n.a.					ρ^{20}	0.9382

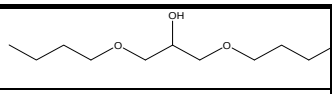
Name	1-*iso*-butoxy-3-methoxy-2-propanol	**Structure**	
Code	4i,0,1		
CAS	635315-52-5		
^{1}H-RMN	0.881, 0.890 (d, 6H); 1.796, 1.813, 1.830, 1.846, 1.863, 1.880, 1.897, 1.913, 1.930 (m, 1H); 2.519 (sa, 1H); 3.208, 3.214, 3.224, 3.231 (dd, 2H); 3.381 (s, 1H); 3.402-3.491 (m, 4H); 3.922, 3.937, 3.949, 3.960, 3.975 (q, 1H)		
^{13}C-RMN	19.169; 28.194; 59.059; 69.219; 71.805; 73.826; 78.264		
FT-IR	1195; 2876; 2926; 2973; 3446		
m/z	162.1		

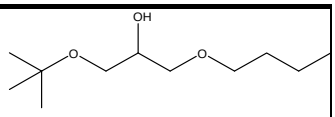
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**	**H**		**O**	**F**	
59.23	11.18		29.59	0.00		58.9	11.0				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.49	**μ**	2.353	**b. p.**	200	n_D^{20}	1.4208	**log P**	0.6007	ν^{20}	n.a.
π*	0.62	**ε**	6.561	ΔH_{vap}^{eb}	50.92	$f_{(dielectric)}$	0.2022	H_2O^{sol}	Miscible	η^{20}	n.a.
α	0.55	$f_{(kirkwood)}$	0.3938	P_{vap}^{298}	n.a.					ρ^{20}	0.9303

Name	1-*tert*-butoxy-3-methoxy-2-propanol	**Structure**	

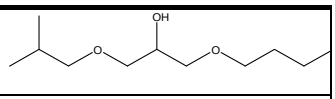
Code	4t,0,1										
CAS	13021-53-9										
^{1}H-RMN	1.180 (s, 9H); 2.578 (sa, 1H); 3.372 (s, 3H); 3.327-3.467 (m, 4H); 3.859 (m, 1H)										
^{13}C-RMN	27.345; 59.032; 62.805; 69.538; 73.042; 73.873										
FT-IR	1114; 1463; 2869; 2924; 2953; 3440										
m/z	162.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
59.23	11.18	29.59	0.00			58.7	11.2				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.44	**μ**	2.359	**b. p.**	195	n_D^{20}	1.4212	**log P**	0.3402	ν^{20}	n.a.
π*	0.71	**ε**	6.612	ΔH_{vap}^{eb}	55.71	$f_{(dielectric)}$	0.2024	H_2O^{sol}	Miscible	η^{20}	n.a.
α	0.36	$f_{(kirkwood)}$	0.3945	P_{vap}^{298}	0.420					ρ^{20}	0.9342

Name	1-*n*-butoxy-3-*iso*-propoxy-2-propanol					**Structure**					
Code	3i,0,4										
CAS	53146-43-3										
^{1}H-RMN	0.875, 0.893, 0.912 (t, 3H); 1.132, 1.147 (d, 6H); 1.295, 1.313, 1.331, 1.350, 1.369, 1.388 (m, 2H); 1.503, 1.520, 1.540, 1.557, 1.574 (q, 2H); 2.585, 2.595 (d, 1H); 3.379-3.492 (m, 6H); 3.547, 3.562, 3.577, 3.592, 3.608 (q,1H); 3.856-3.919 (m, 1H)										
^{13}C-RMN	13.788; 19.149; 31.558; 69.187; 69.479; 71.186; 71.801; 72.018										
FT-IR	1075; 1126; 1374; 1462; 2866; 2931; 2965; 3448										
m/z	190.0										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			63.0	11.8				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.43	**μ**	n.a.	**b. p.**	223	n_D^{20}	n.a.	**log P**	1.4639	ν^{20}	5.053
π*	0.16	**ε**	n.a.	ΔH_{vap}^{eb}	56.93	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	4.590
α	0.77	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	0.9084

Name	1,3-di-*n*-butoxy-2-propanol					**Structure**					
Code	4,0,4										
CAS	2216-77-5										
^{1}H-RMN	0.865, 0.884, 0.902 (t, 3H); 1.286, 1.304, 1.323, 1.342, 1.360, 1.379 (m, 4H); 1.493, 1.510, 1.530, 1.540, 1.548, 1.564 (q, 4H); 2.630 (sa, 1H); 3.381-3.472 (m, 8H); 3.882, 3.895, 3.907, 3.919, 3.933 (q, 1H)										
^{13}C-RMN	13.816; 19.180; 31.582; 69.346; 71.229; 71.791										
FT-IR	1078; 1114; 1461; 2866; 2931; 2956; 3452										
m/z	204.0										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
64.67	11.84	23.49	0.00			64.8	11.5				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.45	**μ**	2.393	**b. p.**	248	n_D^{20}	1.4271	**log P**	2.0663	ν^{20}	6.061
π*	1.09	**ε**	5.642	ΔH_{vap}^{eb}	68.36	$f_{(dielectric)}$	0.2043	H_2O^{sol}	44.7	η^{20}	5.525
α	0.10	$f_{(kirkwood)}$	0.3779	P_{vap}^{298}	0.030					ρ^{20}	0.9117

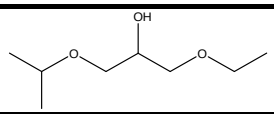
Name	3-*n*-butoxy-1-*tert*-butoxy-2-propanol					**Structure**					
Code	4t,0,4										
CAS	42910-65-6										
^{1}H-RMN	0.872, 0.891, 0.909 (t, 3H); 1.167 (s, 9H); 1.294, 1.312, 1.330, 1.349, 1.368, 1.387 (m, 2H); 1.501, 1.518, 1.537, 1.554, 1.571 (q, 2H); 2.585 (sa, 1H); 3.324-3.479 (m, 6H); 3.808, 3.822, 3.834, 3.845, 3.857, 3.871 (m, 1H)										
^{13}C-RMN	13.820; 19.179; 27.386; 31.603; 62.821; 69.665; 71.193; 71.837; 73.000										
FT-IR	1078; 1116; 1364; 1465; 2871; 2933; 2971; 3457										
m/z	204.0										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
64.67	11.84	23.49	0.00			64.4	11.7				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	

E_T^N	0.39	μ	2.259	b. p.	230	n_D^{20}	1.4257	log P	1.6689	ν^{20}	n.a.
π*	0.75	ε	5.163	ΔH_{vap}^{eb}	44.50	$f_{(dielectric)}$	0.2039	H_2O^{sol}	38.5	η^{20}	n.a.
α	0.22	$f_{(kirkwood)}$	0.3676	P_{vap}^{298}	0.105					ρ^{20}	0.9024

Name	3-*n*-butoxy-1-*iso*-butoxy-2-propanol	**Structure**	
Code	4i,0,4		
CAS	113560-35-3		
^{1}H-RMN	0.873, 0.889 (d, 6H); 0.881, 0.900, 0.919 (t, 3H); 1.302, 1.320, 1.339, 1.357, 1.376, 1.395 (m, 2H); 1.510, 1.527, 1.547, 1.564, 1.580 (q, 2H); 1.804, 1.821, 1.838, 1.854, 1.871, 1.888, 1.904 (m, 1H); 2.544 (sa, 1H); 3.201, 3.218 (d, 2H); 3.407-3.498 (m, 6H); 3.929 (sa,1H)		
^{13}C-RMN	13.815; 19.177; 19.201; 28.235; 31.583; 69.338; 71.219; 71.796; 71.890; 78.277		
FT-IR	1077; 1115; 1465; 2868; 2931; 2956; 3452		
m/z	204.0		

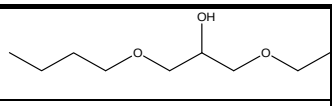
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
64.67	11.84	23.49	0.00	64.4	11.9		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.46	μ	2.257	b. p.	229	n_D^{20}	1.4258	log P	1.9294	ν^{20}	n.a.
π*	0.57	ε	5.149	ΔH_{vap}^{eb}	55.69	$f_{(dielectric)}$	0.2039	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.50	$f_{(kirkwood)}$	0.3672	P_{vap}^{298}	n.a.					ρ^{20}	0.9006

Name	1-ethoxy-3-*iso*-propoxy-2-propanol	**Structure**	
Code	3i,0,2		
CAS	13021-50-6		
^{1}H-RMN	1.131, 1.146 (d, 6H); 1.165, 1.183, 1.200 (t, 3H); 2.608 (s, 1H); 3.377, 3.401, 3.417, 3.439 (c, 2H); 3.458-3.535 (m, 4H); 3.548, 3.563, 3.578, 3.593, 3.609 (q, 1H); 3.885 (m, 1H)		
^{13}C-RMN	14.913; 21.840; 66.589; 69.191; 69.425; 71.646; 71.943		
FT-IR	1076; 1126; 1379; 2869; 2929; 2973; 3437		
m/z	185.1		

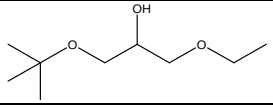
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
59.23	11.18	29.59	0.00	59.0	11.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.45	μ	2.541	b. p.	187	n_D^{20}	1.4176	log P	0.4840	ν^{20}	n.a.
π*	0.75	ε	7.386	ΔH_{vap}^{eb}	26.18	$f_{(dielectric)}$	0.2011	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.36	$f_{(kirkwood)}$	0.4049	P_{vap}^{298}	n.a.					ρ^{20}	0.9338

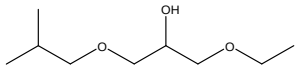
Name	1-*n*-butoxy-3-ethoxy-2-propanol	**Structure**	
Code	4,0,2		
CAS	13021-52-8		
^{1}H-RMN	0.883, 0.902, 0.920 (t, 3H); 1.175, 1.193, 1.210 (t, 3H); 1.304, 1.322, 1.340, 1.359, 1.378, 1.396 (m, 2H); 1.511, 1.528, 1.547, 1.565, 1.582 (q, 2H); 2.555 (sa, 1H); 3.403-3.545 (m, 8H); 3.931 (sa, 1H)		
^{13}C-RMN	13.762; 14.973; 19.143; 31.558; 66.681; 69.332; 71.199; 71.655; 71.818		
FT-IR	1077; 1117; 1460; 2868; 2931; 2958; 3441		
m/z	176.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
61.33	11.44	27.23	0.00	61.1	11.5		

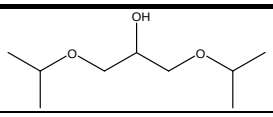
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.45	μ	2.459	b. p.	220	n_D^{20}	1.4237	log P	1.0864	ν^{20}	n.a.
π*	0.96	ε	6.599	ΔH_{vap}^{eb}	44.01	$f_{(dielectric)}$	0.2032	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.21	$f_{(kirkwood)}$	0.3944	P_{vap}^{298}	n.a.					ρ^{20}	0.9277

Name	1-*tert*-butoxy-3-ethoxy-2-propanol	**Structure**	
Code	4t,0,2		
CAS	42910-64-5		
^{1}H-RMN	1.177 (s, 9H); 1.174, 1.191, 1.208 (t, 3H); 2.561, 2.571 (d, 1H); 3.332-3.500 (m, 4H); 3.488, 3.507, 3.524, 3.541 (c, 2H); 3.820-3.885 (m, 1H)		

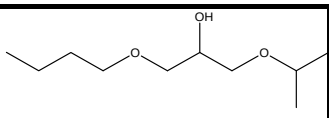
^{13}C-RMN	14.962; 27.331; 62.848; 66.595; 69.638; 71.011; 71.682										
FT-IR	1076; 1116; 1364; 2871; 2929; 2974; 3455										
m/z	176.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
61.33	11.44		27.23	0.00		61.1		11.2			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.41	**μ**	2.317	**b. p.**	204	n_D^{20}	1.4214	**log P**	0.6890	ν^{20}	n.a.
π*	0.62	**ε**	5.965	ΔH_{vap}^{eb}	73.86	$f_{(dielectric)}$	0.2024	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.36	$f_{(kirkwood)}$	0.3840	P_{vap}^{298}	n.a.					ρ^{20}	0.9172

Name	1-*iso*-butoxy-3-ethoxy-2-propanol	**Structure**	
Code	4i,0,2		
CAS	382601-20-9 (patent uses)		
^{1}H-RMN	0.860, 0.876 (d, 6H); 1.161, 1.178, 1.196 (t, 3H); 1.792, 1.808, 1.825, 1.842, 1.859, 1.875, 1.892 (m, 1H); 2.635 (sa, 1H); 3.191, 3.208 (d, 2H); 3.388-3.531 (m, 6H); 3.895, 3.909, 3.921, 3.935, 3.948 (q, 1H)		
^{13}C-RMN	14.997; 19.177; 28.229; 66.694; 69.348; 71.663; 71.931; 78.278		
FT-IR	1076; 1118; 1467; 2869; 2956; 3450		
m/z	176.1		

Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
61.33	11.44		27.23	0.00		61.0		11.2			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.46	**μ**	2.330	**b. p.**	214	n_D^{20}	1.4214	**log P**	0.9495	ν^{20}	n.a.
π*	0.71	**ε**	5.997	ΔH_{vap}^{eb}	40.86	$f_{(dielectric)}$	0.2024	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.40	$f_{(kirkwood)}$	0.3846	P_{vap}^{298}	n.a.					ρ^{20}	0.9134

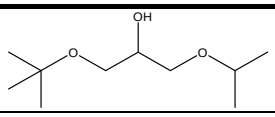
Name	1,3-di-*iso*-propoxy-2-propanol	**Structure**	
Code	3i,0,3i		
CAS	13021-54-0		
^{1}H-RMN	1.118, 1.134 (d, 12H); 2.638 (sa, 1H); 3.372, 3.388, 3.396, 3.411, 3.440, 3.451, 3.463, 3.475 (ddd, 4H); 3.534, 3.549, 3.564, 3.580, 3.595 (q, 2H); 3.813, 3.826, 3.839, 3.851, 3.863 (q, 1H)		
^{13}C-RMN	21.783; 69.126; 69.504; 71.816		
FT-IR	1076; 1129; 1370; 1468; 2870; 2927; 2972; 3450		
m/z	176.0		

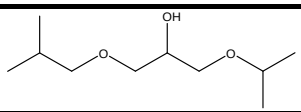
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
61.33	11.44		27.23	0.00		61.5		11.3			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.46	**μ**	n.a.	**b. p.**	202	n_D^{20}	n.d	**log P**	0.8615	ν^{20}	n.a.
π*	n.a.	**ε**	n.a.	ΔH_{vap}^{eb}	40.68	$f_{(dielectric)}$	n.d	H_2O^{sol}	120.8	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	0.480					ρ^{20}	n.d

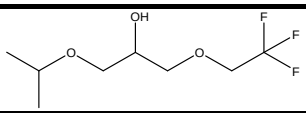
Name	1-*n*-butoxy-3-*iso*-propoxy-2-propanol	**Structure**	
Code	4,0,3i		
CAS	53146-43-3		
^{1}H-RMN	0.881, 0,899, 0.918 (t, 3H); 1.137, 1.152 (d, 6H); 1.301, 1.320, 1.338, 1.357, 1.376, 1.394 (m, 2H); 1.509, 1.526, 1.545, 1.562, 1.579 (q, 2H); 2.583 (sa, 1H); 3.386-3.518 (m, 6H); 3.553, 3.568, 3.583, 3.599, 3.614 (q, 1H); 3.865, 3.880, 3.892, 3.904, 3.918 (q, 1H)		
^{13}C-RMN	13.605; 18.987; 21.735; 31.411; 69.123; 69.307; 70.996; 71.741; 71.825		
FT-IR	1071; 1120; 1371; 1459; 2864; 2927; 2962; 3433		
m/z	290.0		

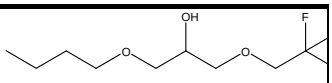
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
63.12	11.65		25.23	0.00		63.1		11.6			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.50	**μ**	2.314	**b. p.**	224	n_D^{20}	1.4238	**log P**	1.4639	ν^{20}	n.a.
π*	1.25	**ε**	5.614	ΔH_{vap}^{eb}	53.32	$f_{(dielectric)}$	0.2032	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.08	$f_{(kirkwoo}$	0.3773	P_{vap}^{298}	n.a.					ρ^{20}	0.9083

		d)									

Name	1-*tert*-butoxy-3-*iso*-propoxy-2-propanol					**Structure**					
Code	4t,0,3i										
CAS	286957-56-0										
^{1}H-RMN	1.130, 1.145 (d, 6H); 1.169 (s, 9H); 2.587 (sa, 1H); 3.330-3.410 (m, 2H); 3.389, 3.401, 3.413, 3.425, 3.447. 3.459, 3.471, 3.483 (ddd, 2H); 3.546, 3.561, 3.576, 3.591, 3.607 (q,1H); 3.805 (m, 1H)										
^{13}C-RMN	21.785; 27.213; 62.708; 69.120; 69.648; 71.730; 72.690										
FT-IR	1073; 1195; 1364; 1468; 2870; 2927; 2971; 3436										
m/z	290.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			63.0	11.8				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.37	**μ**	n.a.	**b. p.**	202	n_D^{20}	n.a.	**log P**	1.0665	ν^{20}	n.a.
π*	0.62	**ε**	n.a.	ΔH_{vap}^{eb}	46.09	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.29	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*iso*-butoxy-3-*iso*-propoxy-2-propanol					**Structure**					
Code	4i,0,3i										
CAS	n.a.										
^{1}H-RMN	0.865, 0.882 (d, 6H); 1.130, 1.146 (d, 6H); 1.797, 1.814, 1.830, 1.847, 1.864, 1.881, 1.897 (m, 1H); 2.591 (sa, 1H); 3.195, 3.212 (d, 2H); 3.388-3.497 (m,4H); 3.546, 3.561, 3.577, 3.592, 3.607 (q, 1H); 3.860, 3.874, 3.887, 3.901, 3.914 (q, 1H)										
^{13}C-RMN	19.059; 21.788; 28.082; 69.143; 69.337; 71.844; 71.860; 78.124										
FT-IR	1075; 1125; 1369; 1467; 2869; 2927; 2967; 3442										
m/z	290.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			62.7	11.5				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.44	**μ**	n.a.	**b. p.**	215	n_D^{20}	n.a.	**log P**	1.3270	ν^{20}	n.a.
π*	0.57	**ε**	n.a.	ΔH_{vap}^{eb}	47.21	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.47	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}						ρ^{20}	n.a.

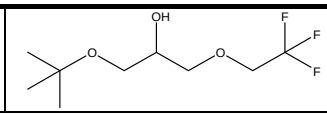
Name	1-*iso*-propoxy-3-(2,2,2-trifluoroethoxy)-2-propanol					**Structure**					
Code	3i,0,3F										
CAS	n.a.										
^{1}H-RMN	1.141, 1.156 (d, 6H); 2.595 (sa, 1H); 3.408, 3.423, 3.431, 3.447, 3.475, 3.486, 3.499, 3.510 (ddd, 2H); 3.562, 3.577, 3.592, 3.607, 3.620 (q, 1H); 3.620, 3.634, 3.644, 3.658, 3.681, 3.693, 3.706, 3.717 (ddd, 2H); 3.851, 3873, 3.895, 3.916 (c,2H); 3.922 (m, 1H)										
^{13}C-RMN	21.743; (68.155, 68.493, 68.831, 69.169 (c)); 68.573; 69.452; 72.148; 73.623; (119.668; 122.446; 125.223; 128.001 (c))										
^{19}F-RMN	-74.28 (t)										
FT-IR	1152; 1280; 1371; 2877; 2933; 2975; 3438										
m/z	216.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
44.44	6.99	22.20	26.36			44.1	7.2		26.0		
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.59	**μ**	3.361	**b. p.**	176	n_D^{20}	1.3821	**log P**	1.1426	ν^{20}	5.087
π*	0.71	**ε**	11.986	ΔH_{vap}^{eb}	37.03	$f_{(dielectric)}$	0.1888	H_2O^{sol}	n.a.	η^{20}	6.895
α	0.54	$f_{(kirkwood)}$	0.4399	P_{vap}^{298}	n.a.					ρ^{20}	1.3556

Name	1-*n*-butoxy-3-(2,2,2-trifluoroethoxy)-2-propanol					**Structure**					
Code	4,0,3F										
CAS	n.a.										
^{1}H-RMN	0.885, 0.903, 0.921 (t, 3H); 1.300, 1.318, 1.336, 1.355, 1.374, 1.393 (m, 2H); 1.508, 1.525, 1.544, 1.561, 1.578 (q, 2H); 2.612 (sa, 1H); 3.414-3.500 (m, 4H); 3.614, 3.629, 3.638, 3.653, 3.680, 3.691, 3.705, 3.716 (ddd, 2H); 3.846,										

	3.868, 3.890, 3.912 (c, 2H); 3.921, 3.933, 3.947, 3.959, 3.972 (q, 1H)
^{13}C-RMN	13.646; 19.076; 31.465; (68.166; 68.505; 68.843; 69.181 (c)); 69.303; 71.205; 71.226; 73.641; (119.736; 122.514; 125.292; 128.070 (c))
^{19}F-RMN	-74.29 (m)
FT-IR	1159; 1278; 1460; 2870; 2932; 2957; 3441
m/z	230.1

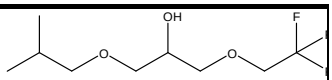
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
46.95	7.44	20.85	24.76	46.5	7.3		24.4

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.60	**μ**	3.446	**b. p.**	210	n_D^{20}	1.3903	**log P**	1.7450	ν^{20}	n.a.
π*	0.84	**ε**	10.235	ΔH_{vap}^{eb}	57.40	$f_{(dielectric)}$	0.1917	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.70	$f_{(kirkwood)}$	0.4301	P_{vap}^{298}	n.a.					ρ^{20}	1.1141

Name	1-*tert*-butoxy-3-(2,2,2-trifluoroethoxy)-2-propanol	**Structure**	
Code	4t,0,3F		
CAS	n.a.		
^{1}H-RMN	1.181 (s, 9H); 2.598 (sa, 1H); 3.359, 3.375, 3.382, 3.397, 3.408, 3.419, 3.430, 3.442 (ddd, 2H); 3.617, 3.631, 3.641, 3.656, 3.679, 3.691, 3.704, 3.716 (ddd, 2H); 3.885 (m, 1H); 3.854, 3.875, 3.897, 3.919 (c, 2H)		
^{13}C-RMN	27.267; 62.206; (68.218; 68.556; 68.894; 69.232 (c)); 69.665; 73.218; 73.616; (119.701; 122.480; 125.258; 128.036 (c))		
^{19}F-RMN	-74.28 (t)		
FT-IR	1152; 1276; 1466; 2874; 2929; 2971; 3440		
m/z	230.1		

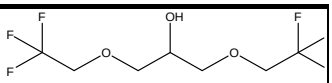
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
46.95	7.44	20.85	24.76	47.1	7.3		24.6

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.57	**μ**	3.642	**b. p.**	199	n_D^{20}	1.3868	**log P**	1.3476	ν^{20}	7.748
π*	0.53	**ε**	11.197	ΔH_{vap}^{eb}	45.79	$f_{(dielectric)}$	0.1905	H_2O^{sol}	n.a.	η^{20}	8.609
α	0.61	$f_{(kirkwood)}$	0.4359	P_{vap}^{298}	n.a.					ρ^{20}	1.1112

Name	1-*iso*-butoxy-3-(2,2,2-trifluoroethoxy)-2-propanol	**Structure**	
Code	4i,0,3F		
CAS	n.a.		
^{1}H-RMN	0.877, 0.894 (d, 6H); 1.805, 1.822, 1.838, 1.855, 1.872, 1.889, 1.905 (m, 1H); 2.567 (sa, 1H); 3.206, 3.214, 3.223, 3.231 (dd, 2H); 3.463 (m, 2H); 3.625, 3.640, 3.649, 3.664, 3.692, 3.703, 3.716, 3.727 (ddd, 2H); 3.850, 3.872, 3.894, 3.916, (c, 2H); 3.928, 3.943, 3.956, 3.968, 3.981 (q, 1H)		
^{13}C-RMN	19.081; 28.204; (68.214; 68.553; 68.891; 69.229 (c)); 69.347; 71.297; 73.647; 78.302 (119.681; 122.460; 125.237; 128.015 (c))		
^{19}F-RMN	-74.28 (t)		
FT-IR	1161; 1278; 1466; 2872; 2930; 2956; 3432		
m/z	230.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
46.95	7.44	20.85	24.76	46.9	7.5		24.5

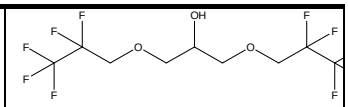
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.60	**μ**	3.431	**b. p.**	205	n_D^{20}	1.3890	**log P**	1.6081	ν^{20}	n.a.
π*	0.57	**ε**	10.013	ΔH_{vap}^{eb}	56.77	$f_{(dielectric)}$	0.1913	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.79	$f_{(kirkwood)}$	0.4287	P_{vap}^{298}	n.a.					ρ^{20}	1.0985

Name	1,3-bis(2,2,2-trifluoroethoxy)-2-propanol	**Structure**	
Code	3F,0,3F		
CAS	691-26-9		
^{1}H-RMN	2.507 (sa, 1H); 3.654, 3.669, 3.678, 3.693, 3.703, 3.714, 3.727, 3.739 (ddd, 4H); 3.853, 3.875, 3.896, 3.918 (c, 4H); 3.957, 3.968, 3.982, 3.995, 4.007, 4.021 (m, 1H)		
^{13}C-RMN	(68.263; 68.603; 68.942; 69.314 (c)); 69.313; 73.071; (119.670; 122.447; 125.224. 128.000 (c))		
^{19}F-RMN	-74.328 (m)		
FT-IR	1157; 1278; 1461; 2891; 2938; 3473		
m/z	256.0		

Theoretical elemental analysis	Experimental elemental analysis

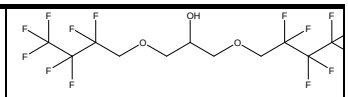
C	H	O	F	C	H	O	F
32.84	3.94	18.74	44.50	32.5	3.8		44.4

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.70	μ	4.098	b. p.	197	n_D^{20}	1.3522	log P	1.4237	ν^{20}	5.883
π*	0.38	ε	14.616	ΔH_{vap}^{eb}	51.00	$f_{(dielectric)}$	0.1779	H_2O^{sol}	28.4	η^{20}	8.140
α	0.82	$f_{(kirkwood)}$	0.4504	P_{vap}^{298}	0.400					ρ^{20}	1.3837

Name	1,3-bis(2,2,3,3,3-pentafluoropropoxy)-2-propanol	Structure	
Code	5F,0,5F		
CAS	935273-12-4		
^{1}H-RMN	2.517 (sa, 1H); 3.657, 3.671, 3.681 (t, 4H), 3.970 (m, 1H); 3.918, 3.950, 3.983 (t, 4H)		
^{13}C-RMN	(67.719, 67.981, 68.224 (t)); 69.248; 73.160; (112.370, 112.741, 113.111, 113.479 (c)); (119.723, 120.070, 120.417 (t))		
^{19}F-RMN	-123.740 (m); -83.804 (m)		
FT-IR	1160; 1250; 1440; 2899; 2943; 3490		
m/z	356.1		

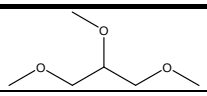
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
30.35	2.83	13.48	53.34	30.1	2.7		53.5

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.70	μ	3.941	b. p.	204	n_D^{20}	1.3354	log P	2.4069	ν^{20}	n.a.
π*	0.56	ε	10.438	ΔH_{vap}^{eb}	43.92	$f_{(dielectric)}$	0.1715	H_2O^{sol}	n.a.	η^{20}	n.a.
α	1.04	$f_{(kirkwood)}$	0.4314	P_{vap}^{298}	n.a.					ρ^{20}	1.3354

Name	1,3-bis(2,2,3,3,4,4,4-heptafluorobutoxy)-2-propanol	Structure	
Code	7F,0,7F		
CAS	1598-17-0		
^{1}H-RMN	2.473, 2.483 (d, 1H); 3.674, 3.687, 3.698 (t, 4H), 3.969 (m, 1H); 3.958, 3.992, 4.026 (t, 4H)		
^{13}C-RMN	(67.862, 68.120, 68.378 (t)); 69.289; 73.247; (114.434, 114.738, 115.039 (t)); (115.892, 116.227, 116.562, 116.890(c)); (118.747, 119.080, 119.416 (t))		
^{19}F-RMN	-127.909 (m); -120.878 (m); -81.174 (t)		
FT-IR	1220; 1457; 2888; 2941; 3480		
m/z	456.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
28.96	2.21	10.52	58.31	28.8	2.3		58.1

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.69	μ	3.903	b. p.	206	n_D^{20}	1.3298	log P	3.3901	ν^{20}	12.554
π*	0.55	ε	8.629	ΔH_{vap}^{eb}	57.57	$f_{(dielectric)}$	0.1694	H_2O^{sol}	n.a.	η^{20}	19.596
α	1.01	$f_{(kirkwood)}$	0.4178	P_{vap}^{298}	n.a.					ρ^{20}	1.5609

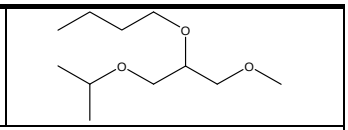
Name	1,2,3-trimethoxypropane	Structure	
Code	1,1,1		
CAS	20637-49-4		
^{1}H-RMN	3.329 (s, 6H); 3.421 (s, 3H); 3.405-3.460 (m, 5H)		
^{13}C-RMN	57.757; 59.146; 72.115; 78.998		
FT-IR	950; 1142; 2890; 2987		
m/z	134.1		

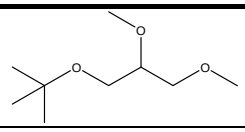
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
53.71	10.52	35.77	0.00	53.9	10.4		

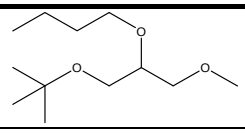
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	2.219	b. p.	150	n_D^{20}	1.4032	log P	-0.1826	ν^{20}	n.a.
π*	n.a.	ε	6.838	ΔH_{vap}^{eb}	30.24	$f_{(dielectric)}$	0.1962	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	0.3978	P_{vap}^{298}	n.a.					ρ^{20}	0.9428

Name	1-*iso*-propoxy-2,3-dimethoxypropane	Structure	

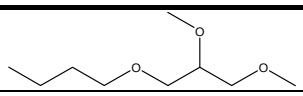
Code	3i,1,1										
CAS	n.a.										
^{1}H-RMN	1.099, 1.104, 1.114, 1.119 (dd, 6H); 3.327 (s, 3H); 3.417 (s, 3H); 3.395-3.476 (m, 5H); 3.500, 3.515, 3.531, 3.546, 3.561 (m, 1H)										
^{13}C-RMN	21.865; 21.932; 57.798; 59.122; 67.301; 72.028; 72.362; 79.353										
FT-IR	923; 961; 1128; 2893; 2972										
m/z	162.1										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
59.23	11.18	29.59	0.00		59.0	11.3					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	n.a.	**μ**	1.993	**b. p.**	170	n_D^{20}	1.4044	**log P**	0.5437	ν^{20}	0.730
π*	n.a.	**ε**	4.918	ΔH_{vap}^{eb}	39.88	$f_{(dielectric)}$	0.1966	H_2O^{sol}	n.a.	η^{20}	1.025
α	n.a.	$f_{(kirkwood)}$	0.3616	P_{vap}^{298}	n.a.					ρ^{20}	1.4044

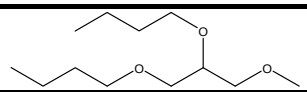
Name	2-*n*-butoxy-3-methoxy-1-*iso*-propoxypropane					**Structure**					
Code	3i,4,1										
CAS	n.a.										
^{1}H-RMN	0.867, 0.885, 0.904 (t, 3H); 1.114, 1.120, 1.129, 1.136 (dd, 6H); 1.297, 1.315, 1.333, 1.352, 1.371, 1.390 (m, 2H); 1.499, 1.516, 1.536, 1.553, 1.570 (q, 2H); 3.344 (s, 3H); 3.390-3.586 (m, 8H)										
^{13}C-RMN	13.851; 19.182; 21.929; 22.054; 32.086; 59.195; 67.811; 70.189; 72.012; 72.831; 77.934										
FT-IR	1126; 2871; 2929; 2966										
m/z	204.2										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
64.67	11.84	23.49	0.00		64.1	11.6					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.15	**μ**	n.a.	**b. p.**	215	n_D^{20}	n.a.	**log P**	1.8724	ν^{20}	n.a.
π*	-0.06	**ε**	n.a.	ΔH_{vap}^{eb}	45.89	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.032	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

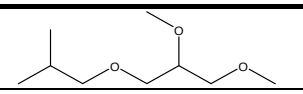
Name	1-*tert*-butoxy-2,3-dimethoxypropane					**Structure**					
Code	4t,1,1										
CAS	172888-77-6										
^{1}H-RMN	1.171 (s, 9H); 3.357 (s, 3H); 3.416 (sa, 4H); 3.450 (s, 3H); 3.487-3.533 (m, 1H)										
^{13}C-RMN	27.393; 57.953; 50.179; 60.952; 72.540; 72.957; 79.728										
FT-IR	1098 2877; 2904; 2929; 2974										
m/z	176.1										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
61.33	11.44	27.23	0.00		61.0	11.1					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.21	**μ**	n.a.	**b. p.**	180	n_D^{20}	n.a.	**log P**	180	ν^{20}	n.a.
π*	0.53	**ε**	n.a.	ΔH_{vap}^{eb}	34.63	$f_{(dielectric)}$	n.a.	H_2O^{sol}	21.2	η^{20}	n.a.
α	0.02	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	0.751					ρ^{20}	n.a.

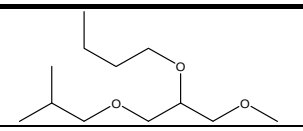
Name	2-*n*-butoxy-1-*tert*-butoxy-3-methoxypropane					**Structure**					
Code	4t,4,1										
CAS	n.a.										
^{1}H-RMN	0.873, 0.892, 0.910 (t, 3H); 1.163 (s, 9H); 1.304, 1.322, 1.341, 1.360, 1.378, 1.397 (m, 2H); 1.505, 1.521, 1.541, 1.559, 1.576 (q, 2H); 3.349 (s, 3H); 3.386-3.419 (m, 3H); 3.448-3.518 (m, 2H); 3.544, 3.561, 3.578 (t, 2H)										
^{13}C-RMN	13.877; 19.204; 27.414; 32.108; 59.190; 61.417; 70.241; 72.893; 78.188										
FT-IR	1106; 2872; 2929; 2970										
m/z	218.2										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
66.01	12.00	21.98	0.00		65.8	11.9					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	

E_T^N	n.a.	μ	n.a.	b. p.	219	n_D^{20}	n.a.	log P	2.0774	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	46.77	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

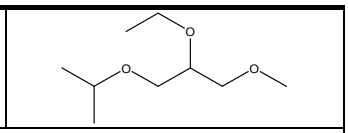
Name	1-*n*-butoxy-2,3-dimetoxypropane					Structure					
Code	4,1,1										
CAS	n.a.										
^{1}H-RMN	0.869, 0.887, 0.905 (t, 3H); 1.290, 1.308, 1.327, 1.346, 1.365, 1.383 (m, 2H); 1.394, 1.511, 1.530, 1.548, 1.566 (q, 2H); 3.346 (s, 3H); 3.405-3.489 (m, 7H); 3.439 (s, 3H)										
^{13}C-RMN	13.830; 19.205; 31.612; 57.857; 59.184; 70.072; 71.306; 72.397; 79.174										
FT-IR	1194; 2872; 2900; 2932; 2956										
m/z	176.1										
Theoretical elemental analysis						Experimental elemental analysis					
C	H	O	F			C	H	O	F		
61.33	11.44	27.23	0.00			60.9	11.6				
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.18	μ	n.a.	b. p.	199	n_D^{20}	n.a.	log P	n.a.	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	59.08	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

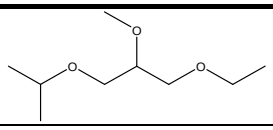
Name	1,2-di-*n*-butoxy-3-methoxypropane					Structure					
Code	4,4,1										
CAS	n.a.										
^{1}H-RMN	0.881, 0.885, 0.899, 0.904, 0.917, 0.922 (dt, 6H); 1.308, 1.326, 1.344, 1.363, 1.382, 1.401 (m, 4H); 1.503, 1.519, 1.532, 1.551, 1.568, 1.586 (q, 4H); 3.358 (s, 3H); 3.407, 3.421, 3.432 (t, 2H); 3.438-3.524 (m, 5H); 3.546, 3.562, 3.579 (t, 2H)										
^{13}C-RMN	13.887; 19.219; 19.260; 31.704; 32.117; 59.242; 70.221; 70.556; 71.289; 72.84; 77.718										
FT-IR	1115; 2868; 2930; 2955										
m/z	218.2										
Theoretical elemental analysis						Experimental elemental analysis					
C	H	O	F			C	H	O	F		
66.01	12.00	21.08	0.00			65.8	12.2				
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	234	n_D^{20}	n.a.	log P	2.4748	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	59.08	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

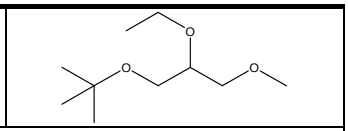
Name	1-*iso*-butoxy-2,3-dimethoxypropane					Structure					
Code	4i,1,1										
CAS	n.a.										
^{1}H-RMN	0.869, 0.871, 0.886, 0.888 (dd, 6H); 1.802, 1.819, 1.835, 1.852, 1.869, 1.886, 1.902 (m, 1H); 3.180, 3.186, 3.197, 3.203 (dd, 2H); 3.359 (s, 3H); 3.454 (s, 3H); 3.460-3.514 (m, 5H)										
^{13}C-RMN	19.254; 28.269; 57.932; 59.222; 70.248; 72.491;78.442; 79.197										
FT-IR	1112; 2871; 2894; 2926; 2953										
m/z											
Theoretical elemental analysis						Experimental elemental analysis					
C	H	O	F			C	H	O	F		
61.33	11.44	27.23	0.00			61.1	11.5				
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	193	n_D^{20}	n.a.	log P	1.0092	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	51.20	$f_{(dielectric)}$	n.a.	H_2O^{sol}	12.2	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	2-*n*-butoxy-1-*iso*-butoxy-3-methoxypropane	Structure	
Code	4i,4,1		
CAS	n.a.		
^{1}H-RMN	0.872, 0.889 (d, 6H); 0.879, 0898, 0.916 (t, 3H); 1.309, 1.327, 1.345, 1.364, 1.383, 1.402 (m, 1H); 1.332, 1.351, 1.369, 1.388 (m, 1H); 1.513, 1.530, 1.550, 1.567, 1.584 (q, 2H); 1.780, 1.797, 1.813, 1.830, 1.847, 1.864, 1.880, 1.897, 1.914 (m, 1H); 3.187, 3.304 (d, 2H); 3.357 (s, 3H), 3.410-3.505 (m, 4H); 3.531-3.582 (m, 3H)		

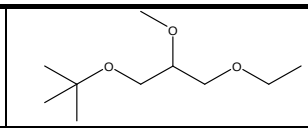
^{13}C-RMN	13.886; 19.219; 19.280; 28.320; 32.120; 59.238; 70.234; 70.733; 72.870; 77.697; 78.401										
FT-IR	1114; 2870; 2929; 2956										
m/z	218.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
66.01	12.00		21.98	0.00		65.9		12.2			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	n.a.	**μ**	n.a.	**b. p.**	227	n_D^{20}	n.a.	**log P**	2.3379	ν^{20}	n.a.
π*	n.a.	**ε**	n.a.	ΔH_{vap}^{eb}	50.63	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

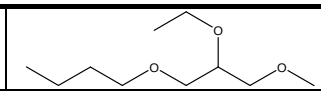
Name	2-ethoxy-3-methoxy-1-*iso*-propoxypropane						**Structure**				
Code	3i,2,1										
CAS	n.a.										
^{1}H-RMN	1.136, 1.142, 1.152, 1.158 (dd, 6H); 1.185, 1.202, 1.220 (t, 3H); 3.368 (s, 3H); 3.415-3.592 (m, 6H); 3.613, 3.618, 3.631, 3.636, 3.648, 3.653, 3.666, 3.671 (dc, 2H)										
^{13}C-RMN	15.611; 21.988; 22.098; 59.259; 65.646; 67.850; 72.098; 72.922; 77.759										
FT-IR	1111; 2873; 2971										
m/z	176.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
61.33	11.44		27.23	0.00		61.1		11.1			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.17	**μ**	n.a.	**b. p.**	161	n_D^{20}	n.a.	**log P**	0.8925	ν^{20}	n.a.
π*	-0.02	**ε**	n.a.	ΔH_{vap}^{eb}	26.02	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.35	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

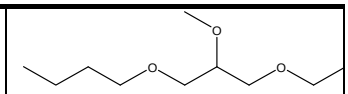
Name	3-ethoxy-2-methoxy-1-*iso*-propoxypropane						**Structure**				
Code	3i,1,2										
CAS	n.a.										
^{1}H-RMN	1.115, 1.119, 1.130, 1.134 (dd, 6H); 1.153, 1.170, 1.188 (t, 3H); 3.434 (s, 3H); 3.460-3.579 (m, 8H)										
^{13}C-RMN	15.051; 21.919; 21.978; 57.858; 66.721; 67.481; 70.095; 72.032; 79.533										
FT-IR	1127; 2867; 2900; 2931; 2973										
m/z	176.1										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
61.33	11.44		27.23	0.00		61.0		11.5			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.17	**μ**	n.a.	**b. p.**	183	n_D^{20}	n.a.	**log P**	0.8925	ν^{20}	n.a.
π*	0.15	**ε**	n.a.	ΔH_{vap}^{eb}	48.72	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.22	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

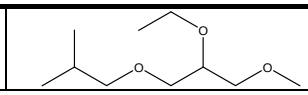
Name	1-*tert*-butoxy-2-ethoxy-3-methoxypropane						**Structure**				
Code	4t,2,1										
CAS	n.a.										
^{1}H-RMN	1.174 (s, 9H); 1.179, 1.197, 1.215 (t, 3H); 3.363 (s, 3H); 3.400-3.440 (m, 3H); 3.181-3.535 (m, 2H); 3.629, 3.637, 3.646, 3.654 (dd, 2H)										
^{13}C-RMN	15.605; 27.435; 59.224; 61.392; 65.659; 72.930; 72.966; 77.981										
FT-IR	1114; 2873; 2901; 2925; 2973										
m/z	190.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**		**O**	**F**		**C**		**H**		**O**	**F**
63.12	11.65		25.23	0.00		62.5		11.9			
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	n.a.	**μ**	n.a.	**b. p.**	190	n_D^{20}	n.a.	**log P**	1.0975	ν^{20}	n.a.
π*	n.a.	**ε**	n.a.	ΔH_{vap}^{eb}	43.99	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwoo}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

		d)									

Name	1-*tert*-butoxy-3-ethoxy-2-methoxypropane					**Structure**					
Code	4t,1,2										
CAS	n.a.										
^{1}H-RMN	1.163, 1.180, 1.197 (t, 3H); 1.165 (s, 9H); 3.443 (s, 3H); 3.415-3.560 (m, 7H)										
^{13}C-RMN	15.097; 27.378; 57.941; 60.927; 66.705; 70.142; 72.892; 79.784										
FT-IR	1117; 2869; 2905; 2929; 2973										
m/z	190.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			62.8	11.9				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.15	**μ**	n.a.	**b. p.**	193	n_D^{20}	n.a.	**log P**	1.0975	ν^{20}	n.a.
π*	-0.23	**ε**	n.a.	ΔH_{vap}^{eb}	43.18	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.47	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	1.0975					ρ^{20}	n.a.

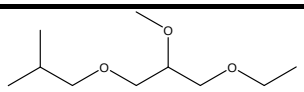
Name	1-*n*-butoxy-2-ethoxy-3-methoxypropane					**Structure**					
Code	4,2,1										
CAS	n.a.										
^{1}H-RMN	0.877, 0.895, 0.914 (t, 3H); 1.170, 1.188, 1.205 (t, 3H), 1.298, 1.317, 1.335, 1.354, 1.373, 1.391 (m, 2H); 1.496, 1.513, 1.533, 1.551, 1.567 (q, 2H); 3.350 (s, 3H); 3.403-3.502 (m, 6H); 3.538, 3.552, 3.564, 3.575 (c, 1H); 3.596, 3.599, 3.613, 3.617, 3.630, 3.635, 3.648, 3.652 (dc, 2H)										
^{13}C-RMN	13.858; 15.564; 19.235; 31.668; 59.209; 65.596; 70.528; 71.280; 72.841; 77.472										
FT-IR	1121; 2811; 2970; 2929; 2959										
m/z	190.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			62.8	11.2				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.16	**μ**	n.a.	**b. p.**	209	n_D^{20}	n.a.	**log P**	n.a.	ν^{20}	n.a.
π*	0.10	**ε**	n.a.	ΔH_{vap}^{eb}	51.60	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.23	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*n*-butoxy-3-ethoxy-2-methoxypropane					**Structure**					
Code	4,1,2										
CAS	346705-85-9										
^{1}H-RMN	0.882, 0.901, 0,919 (t, 3H); 1.172, 1.189, 1.207 (t, 3H); 1.305, 1.323, 1.341, 1.360, 1.379, 1.398 (m, 2H); 1.510, 1.526, 1.547, 1.563, 1.581 (q, 2H); 3.421-3.550 (m, 9H); 3.455 (s, 3H)										
^{13}C-RMN	13.873; 15.095; 19.246; 31.659; 57.925; 66.795; 70.160; 70.278; 71.328; 79.354										
FT-IR	1117; 2868; 2900; 2932; 2958										
m/z	190.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		
63.12	11.65	25.23	0.00			63.0	11.7				
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.16	**μ**	n.a.	**b. p.**	209	n_D^{20}	n.a.	**log P**	1.4949	ν^{20}	n.a.
π*	0.16	**ε**	n.a.	ΔH_{vap}^{eb}	52.78	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.21	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*iso*-butoxy-2-ethoxy-3-methoxypropane					**Structure**					
Code	4i,2,1										
CAS	n.a.										
^{1}H-RMN	0.877, 0.894 (d, 6H); 1.182, 1.199, 1.217 (t, 3H); 1.819, 1.836, 1.853, 1.869, 1.886 (m, 1H); 3.192, 3.209 (d, 2H); 3.363 (s, 3H); 3.420-3.510 (m, 4H); 3.557, 3.571, 3.584, 3.595 (c, 1H); 3.627, 3.635, 3.645, 3.652 (dd, 2H)										
^{13}C-RMN	15.601; 19.285, 28.311; 59.248; 65.654; 70.725; 72.910; 77.470; 78.44										
FT-IR	1115; 2893; 2928; 2957; 2970										
m/z	190.2										
Theoretical elemental analysis						**Experimental elemental analysis**					
C	**H**	**O**	**F**			**C**	**H**	**O**	**F**		

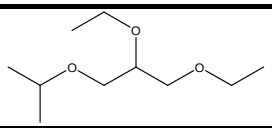
63.12	11.65	25.23	0.00	63.0	11.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	198	n_D^{20}	n.a.	log P	1.3580	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	45.99	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*iso*-butoxy-3-ethoxy-2-methoxypropane	**Structure**	
Code	4i,1,2		
CAS	n.a.		
^{1}H-RMN	0.840, 0.857 (d, 6H); 1.139, 1.157, 1.174 (t, 3H); 1.774, 1.790, 1.807, 1.824, 1.841, 1.857, 1.874 (m, 1H); 3.152, 3.158, 3.169, 3.175 (dd, 2H); 3.424 (s, 3H); 3.438-3.525 (m, 7H)		
^{13}C-RMN	15.011; 19.186; 28.207; 57.867; 66.702; 70.154; 70.361; 78.355; 79.277		
FT-IR	1117; 2869; 2895; 2929; 2955		
m/z	190.2		

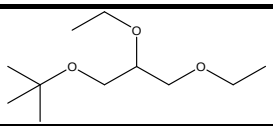
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
63.12	11.65	25.23	0.00	62.1	11.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.16	μ	n.a.	b. p.	201	n_D^{20}	n.a.	log P	1.3580	ν^{20}	n.a.
π*	0.32	ε	n.a.	ΔH_{vap}^{eb}	51.59	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.07	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	2,3-diethoxy-1-*iso*-propoxypropane	**Structure**	
Code	3i,2,2		
CAS	n.a.		
^{1}H-RMN	1.123, 1.128, 1.138, 1.144 (dd, 6H); 1.160, 1.167, 1.178, 1.184, 1.195, 1.202 (dt, 6H); 3.428-3.533 (m, 6H); 3.520, 3.535, 3.550, 3.566, 3.581, 3.596 (m, 2H); 3.608, 3.625, 3.643, 3.660 (c, 2H)		
^{13}C-RMN	15.115; 15.589; 21.967; 22.068; 65.629; 66.729; 67.987; 70.569; 72.022; 77.854		
FT-IR	1120; 2867; 2973		
m/z	190.2		

Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
63.12	11.65	25.23	0.00	63.0	11.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	1192	n_D^{20}	n.a.	log P	1.2413	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	43.90	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

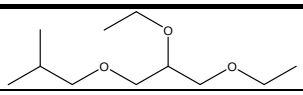
Name	1-*tert*-butoxy-2,3-diethoxypropane	**Structure**	
Code	4t,2,2		
CAS	n.a.		
^{1}H-RMN	1.162 (s, 9H); 1.158, 1.163, 1.176, 1.180, 1.193, 1.198 (dt, 6H); 3.392-3.559 (m, 7H); 3.609, 3.626, 3.644, 3.661 (c, 2H)		
^{13}C-RMN	15.129; 15.580; 27.422; 61.506; 65.641; 66.684; 70.623; 72.866; 78.077		
FT-IR	1114; 2869; 2900; 2929; 2973		
m/z	204.2		

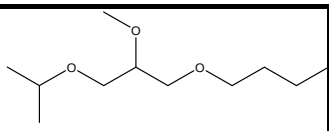
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
64.67	11.84	23.49	0.00	64.1	12.0		

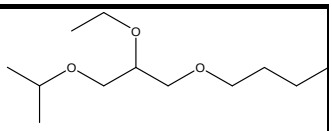
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.16	μ	n.a.	b. p.	199	n_D^{20}	n.a.	log P	1.4463	ν^{20}	n.a.
π*	-0.17	ε	n.a.	ΔH_{vap}^{eb}	37.39	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.44	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*n*-butoxy-2,3-diethoxypropane	**Structure**	
Code	4,2,2		

CAS	382601-24-3										
^{1}H-RMN	0.873, 0.892, 0.910 (t, 3H); 1.155, 1.164, 1.173, 1.181, 1.190, 1.199 (dt. 6H); 1.296, 1.314, 1.332, 1.351, 1.370, 1.389 (m, 2H); 1.494, 1.511, 1.531, 1.548, 1.564 (q, 2H); 3.413-3.522 (m, 8H); 3.536, 3.549, 3.562, 3.574 (c, 1H); 3.602, 3.619, 3.637, 3.654 (c, 2H)										
^{13}C-RMN	13.861; 15.095; 15.574; 19.235; 31.674; 65.618; 66.734; 70.546; 70.716; 71.252; 77.606										
FT-IR	1114; 2861; 2927; 2959										
m/z	204.2										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
64.67	11.84	23.49	0.00		65.0	11.2					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.16	**μ**	n.a.	**b. p.**	217	n_D^{20}	n.a.	**log P**	1.8437	ν^{20}	n.a.
π*	0.15	**ε**	n.a.	ΔH_{vap}^{eb}	49.93	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.211	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

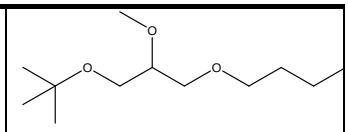
Name	1-*iso*-butoxy-2,3-diethoxypropane					**Structure**					
Code	4i,2,2										
CAS	n.a.										
^{1}H-RMN	0.877, 0.894 (d, 6H);1.173, 1.181, 1.190, 1.198, 1.208, 1.216 (dt, 6H); 1.807, 1.823, 1.840, 1.857, 1.874, 1.890, 1.907 (m, 1H); 3.194, 3.198, 3.211, 3.215 (dd, 2H); 3.440-3.547 (m, 6H); 3.561, 3.574, 3.587, 3.599 (c, 1H); 3.623, 3.641, 3.658, 3.676 (c, 2H)										
^{13}C-RMN	15.140; 15.623; 19.304; 28.316; 65.694; 66.778; 70.640; 70.933; 77.613; 78.406										
FT-IR	1114; 2869; 2897; 2958; 2973										
m/z	204.2										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
64.67	11.84	23.49	0.00		64.5	11.9					
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	n.a.	**μ**	n.a.	**b. p.**	210	n_D^{20}	n.a.	**log P**	1.7068	ν^{20}	n.a.
π*	0.41	**ε**	n.a.	ΔH_{vap}^{eb}	54.18	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	1-*n*-butoxy-2-methoxy-3-*iso*-propoxypropane					**Structure**					
Code	3i,1,4										
CAS	n.a.										
^{1}H-RMN	0.844, 0.862, 0.880 (t, 3H); 1.098, 1.113 (d, 6H); 1.269, 1.288, 1.308, 1.326, 1.344, 1.362 (m, 2H); 1.472, 1.493, 1.510, 1.527, 1.544 (q, 2H); 3.383-3.543 (m, 8H); 3.410 (s, 3H)										
^{13}C-RMN	13.781; 19.170; 21.877; 21.931; 31.598; 57.831; 67.510; 70.250; 71.203; 71.970; 79.490										
FT-IR	1122; 2905; 2931; 2968										
m/z	204.2										
Theoretical elemental analysis					**Experimental elemental analysis**						
C	**H**	**O**	**F**		**C**	**H**	**O**	**F**			
64.67	11.84	23.49	0.00								
Polarity				**Vaporization**		**Polarizability**		**Hydrophobicity**		**Others**	
E_T^N	0.16	**μ**	2.175	**b. p.**	218	n_D^{20}	1.4135	**log P**	1.8724	ν^{20}	1.865
π*	0.31	**ε**	4.800	ΔH_{vap}^{eb}	61.87	$f_{(dielectric)}$	0.1998	H_2O^{sol}	8.1	η^{20}	1.669
α	0.07	$f_{(kirkwood)}$	0.3585	P_{vap}^{298}	n.a.					ρ^{20}	0.8952

Name	1-*n*-butoxy-2-ethoxy-3-*iso*-propoxypropane					**Structure**					
Code	3i,2,4										
CAS	n.a.										
^{1}H-RMN	0.849, 0.868, 0.886 (t, 3H); 1.093, 1.098, 1.108, 1.113 (dd, 6H); 1.134, 1.151, 1.169 (t, 3H); 1.274, 1.293, 1.311, 1.330, 1.349, 1.367 (m, 2H); 1.472, 1.488, 1.507, 1.525, 1.541 (q, 2H); 3.390-3.548 (m, 8H); 3.577, 3.595, 3.612, 3.630 (c, 2H)										
^{13}C-RMN	13.799; 15.516; 19.190; 21.891; 21.987; 31.644; 65.570; 67.996; 70.756; 71.171; 71.931; 77.796										
FT-IR	1122; 2867; 2909; 2931; 2969										
m/z	218.2										
Theoretical elemental analysis					**Experimental elemental analysis**						

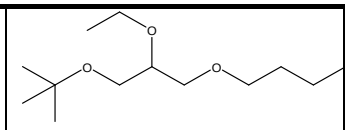
C	H	O	F	C	H	O	F
66.01	12.00	21.98	0.00	66.6	12.2		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	222	n_D^{20}	n.a.	log P	2.2212	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	51.57	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	3-*n*-butoxy-1-*tert*-butoxy-2-methoxypropane	Structure	
Code	4t,1,4		
CAS	n.a.		
^{1}H-RMN	0.850, 0.868, 0.887 (t, 3H); 1.140 (s, 9H); 1.277, 1.295, 1.314, 1.333, 1.351, 1.369 (m, 2H); 1.481, 1.497, 1.519, 1.536, 1.553 (q, 2H); 3.375-3.437 (m, 6H); 3.417 (s, 3H); 3.490-3.522 (m, 1H)		
^{13}C-RMN	13.810; 19.194; 27.331; 31.645; 57.907; 61.006; 70.353; 71.198; 72.775; 79.767		
FT-IR	1118; 2869; 2903; 2931; 2956		
m/z	218.2		

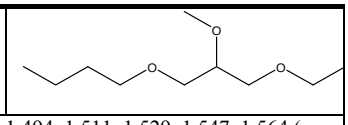
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
66.01	12.00	21.98	0.00	65.3	12.4		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.14	μ	n.a.	b. p.	234	n_D^{20}	n.a.	log P	2.0774	ν^{20}	n.a.
π*	0.42	ε	n.a.	ΔH_{vap}^{eb}	63.06	$f_{(dielectric)}$	n.a.	H_2O^{sol}	5.3	η^{20}	n.a.
α	-0.04	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	3-*n*-butoxy-1-*tert*-butoxy-2-ethoxypropane	Structure	
Code	4t,2,4		
CAS	n.a.		
^{1}H-RMN	0.857, 0.875, 0.894 (t, 3H); 1.149 (s, 9H); 1.139, 1.157, 1.175 (t, 3H); 1.282, 1.300, 1.319, 1.338, 1.357, 1.375 (m, 2H); 1.482, 1.498, 1.519, 1.536, 1.553 (q, 2H); 3.367-3.525 (m, 7H); 3.589, 3.607, 3.624, 3.642 (c, 2H)		
^{13}C-RMN	13.844; 15.539; 19.221; 27.377; 31.692; 61.563; 65.613; 70.878; 71.179; 72.780; 78.045		
FT-IR	1119; 2869; 2931; 2972		
m/z	232.2		

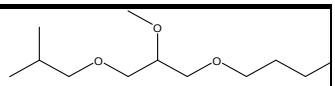
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
67.20	12.15	20.66	0.00	67.0	12.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	211	n_D^{20}	n.a.	log P	2.4262	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	60.04	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	

Name	1,3-di-*n*-butoxy-2-methoxypropane	Structure	
Code	4,1,4		
CAS	n.a.		
^{1}H-RMN	0.866, 0.885, 0.903 (t, 6H); 1.290, 1.308, 1.327; 1.345; 1.364; 1.383 (m, 4H); 1.494, 1.511, 1.529, 1.547, 1.564 (q, 4H); 3.435 (s, 3H); 3.402-3.521 (m, 9H)		
^{13}C-RMN	13.828; 19.214; 31.632; 57.893; 70.302; 71.276; 79.314;		
FT-IR	1118; 2866; 2931; 2957		
m/z	218.2		

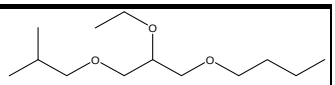
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
66.01	12.00	21.98	0.00	65.8	12.0		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.15	μ	2.184	b. p.	244	n_D^{20}	1.4191	log P	2.4748	ν^{20}	4.316
π*	0.24	ε	4.680	ΔH_{vap}^{eb}	48.78	$f_{(dielectric)}$	0.2017	H_2O^{sol}	4.4	η^{20}	3.783
α	0.10	$f_{(kirkwood)}$	0.3552	P_{vap}^{298}						ρ^{20}	0.8765

Name	3-*n*-butoxy-1-*iso*-butoxy-2-methoxypropane	**Structure**	
Code	4i,1,4		
CAS	n.a.		
^{1}H-RMN	0.850, 0.867 (d, 6H); 0.858, 0.877, 0.895 (t, 3H); 1.283, 1.301, 1.319, 1.339, 1.357, 1.376 (m, 2H); 1.486, 1.503, 1.522, 1.540, 1.557 (q, 2H); 1.782, 1.799, 1.816, 1.832, 1.849, 1.866, 1.882 (m, 1H); 3.158, 3.164, 3.175, 3.181 (dd, 2H); 3.395-3.506 (m, 7H); 3.430 (s, 3H)		
^{13}C-RMN	13.812; 19.209; 28.237; 31.623; 57.915; 70.370; 70.449; 71.257; 78.380; 79.305		
FT-IR	1098; 1116; 2869; 2931; 2971		
m/z	218.2		

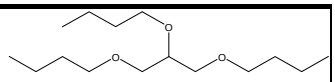
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
66.01	12.00	21.98	0.00	66.3	11.5		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.15	**μ**	n.a.	**b. p.**	226	n_D^{20}	n.a.	**log P**	2.3379	ν^{20}	n.a.
π*	0.39	**ε**	n.a.	ΔH_{vap}^{eb}	51.86	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	0.00	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	3-*n*-butoxy-1-*iso*-butoxy-2-ethoxypropane	**Structure**	
Code	4i,2,4		
CAS	n.a.		
^{1}H-RMN	0.816, 0.833 (d, 6H); 0.826, 0.844, 0.862 (t, 3H); 1.111, 1.128, 1.146 (t, 3H); 1.251, 1.269, 1.288, 1.307, 1.325, 1.344 (m, 2H); 1.447, 1.464, 1.483, 1.501, 1.517 (q, 2H); 1.743, 1.759, 1.776, 1.792, 1.809, 1.826, 1.842 (m, 1H); 3.129, 3.146 (d, 2H), 3.363-3.467 (m, 6H); 3.493, 3.505, 3.518, 3.531 (c, 1H); 3.556, 3.574, 3.591, 3.609 (c, 2H)		
^{13}C-RMN	13.739; 15.458; 19.142; 28.195; 31.590; 65.544; 70.727; 70.855; 71.123; 77.496; 78.250;		
FT-IR	1116; 2867; 2901; 2930; 2957		
m/z	232.2		

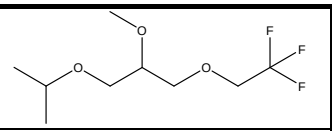
Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
67.20	12.15	20.66	0.00	67.0	12.2		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	**μ**	n.a.	**b. p.**	241	n_D^{20}	n.a.	**log P**	2.6867	ν^{20}	n.a.
π*	n.a.	**ε**	n.a.	ΔH_{vap}^{eb}	63.32	$f_{(dielectric)}$	n.a.	H_2O^{sol}	n.a.	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

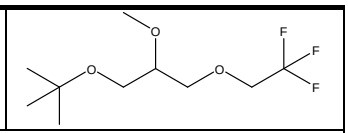
Name	1,2,3-tri-*n*-butoxypropane	**Structure**	
Code	4,4,4		
CAS	131570-29-1		
^{1}H-RMN	0.880, 0.899, 0.917 (t, 3H); 0.885, 0.903, 0.921 (t, 6H); 1.307, 1.326, 1.344, 1.363, 1.382, 1.400 (m, 6H); 1.503, 1.520, 1.540, 1.558, 1.574 (q, 6H); 3.420-3.585 (m, 11H)		
^{13}C-RMN	13.895; 19.226; 19.273; 31.728; 32.139; 70.808; 70.231; 71.273; 77.858;		
FT-IR	1122; 2867; 2932; 2957		
m/z	260.2		

Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
69.18	12.39	18.43	0.00	69.0	12.5		

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	**μ**	2.39	**b. p.**	270	n_D^{20}	1.4237	**log P**	3.8035	ν^{20}	3.151
π*	1.12	**ε**	4.700	ΔH_{vap}^{eb}	77.06	$f_{(dielectric)}$	0.2032	H_2O^{sol}	2.3	η^{20}	2.721
α	n.a.	$f_{(kirkwood)}$	0.3558	P_{vap}^{298}	n.a.					ρ^{20}	0.8636

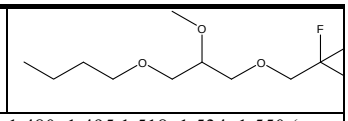
Name	3-*iso*-propoxy-2-methoxy-1-(2,2,2-trifluoroethoxy)-propane	**Structure**	
Code	3i,1,3F		
CAS	n.a.		
^{1}H-RMN	1.095, 1.110 (d, 6H); 3.408 (sa, 3H); 3.448 (sa, 3H); 3.494, 3.510, 3.525, 3.540, 3.555 (q, 1H); 3.618, 3.628, 3.644, 3.655 (dd, 1H); 3.723, 3.749 (d, 1H); 3.800, 3.822, 3.844, 3.866 (c, 2H)		
^{13}C-RMN	21.766; 21.837; 57.852; 66.528; (68.287, 68.624, 68.962, 69.299 (c)); 72.123; 72.244; 79.445; (119.752, 122.531, 125.310, 128.089 (c))		
^{19}F-RMN	-74.334 (m)		
FT-IR	1120; 1281; 2890; 2925; 2973		

m/z	230.1									
Theoretical elemental analysis					Experimental elemental analysis					
C	H	O	F		C	H	O	F		
46.95	7.44	20.85	24.76		46.7	7.6		24.4		
Polarity				Vaporization		Polarizability		Hydrophobicity		Others
E_T^N	n.a.	μ	3.506	b. p.	180	n_D^{20}	1.3748	log P	1.5511	ν^{20}	n.a.
π*	0.88	ε	9.938	ΔH_{vap}^{eb}	39.23	$f_{(dielectric)}$	0.1862	H_2O^{sol}	4.5	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	0.4281	P_{vap}^{298}	n.a.					ρ^{20}	1.0672

Name	3-*tert*-butoxy-2-methoxy-1-(2,2,2-trifluoroethoxy)-propane	Structure	
Code	4t,1,3F		
CAS	n.a.		
^{1}H-RMN	1.158 (s, 9H); 3.415 (sa, 3H); 3.435 (s, 3H); 3.632, 3.643, 3.662, 3.668 (dd, 1H); 3.749, 3.755, 3.779, 3.785 (dd, 1H); 3.827, 3.849, 3.871, 3.893 (c, 2H)		
^{13}C-RMN	27.285; 57.980; 60.133; (68.353, 68.690, 69.027, 69.364 (c)); 72.346; 73.020; 79.763; (119.848; 122.574; 125.353; 128.217 (c))		
^{19}F-RMN	-74.384; -74.361; -74.337		
FT-IR	1126; 1277; 2881; 2930; 2972		
m/z	244.1		

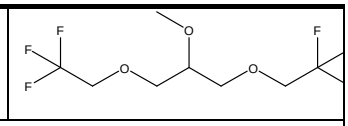
Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
49.17	7.84	19.65	23.33	49.3	7.8		23.1

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.37	μ	3.484	b. p.	185	n_D^{20}	1.3816	log P	1.7561	ν^{20}	2.046
π*	0.69	ε	9.266	ΔH_{vap}^{eb}	47.19	$f_{(dielectric)}$	0.1886	H_2O^{sol}	4.4	η^{20}	2.139
α	0.24	$f_{(kirkwood)}$	0.4232	P_{vap}^{298}	n.a.					ρ^{20}	1.0456

Name	3-*n*-butoxy-2-methoxy-1-(2,2,2-trifluoroethoxy)propane	Structure	
Code	4,1,3F		
CAS	n.a.		
^{1}H-RMN	0.849, 0.867, 0.886 (t, 3H); 1.278, 1.298, 1.312, 1.334, 1.350, 1.370 (m, 2H); 1.480, 1.495 1.518, 1.534, 1.550 (q, 2H); 3.335-3.537 (m, 9H); 3.237 (s, 3H)		
^{13}C-RMN	13.883; 19.269; 31.730; 57.210; (69.838; 70.175; 70.512; 70.849 (c)); 71.701; 72.052; 82.128; (119.756; 122.482; 125.262; 128.122 (c))		
^{19}F-RMN	-74.351		
FT-IR	1120; 1298; 2865; 2922; 2950		
m/z	244.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
49.17	7.84	19.65	23.33	49.5	7.9		23.2

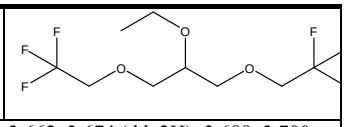
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	n.a.	μ	n.a.	b. p.	207	n_D^{20}	n.a.	log P	2.1535	ν^{20}	n.a.
π*	n.a.	ε	n.a.	ΔH_{vap}^{eb}	42.23	$f_{(dielectric)}$	n.a.	H_2O^{sol}	4.1	η^{20}	n.a.
α	n.a.	$f_{(kirkwood)}$	n.a.	P_{vap}^{298}	n.a.					ρ^{20}	n.a.

Name	2-methoxy-1,3-bis(2,2,2-trifluoroethoxy)propane	Structure	
Code	3F,1,3F		
CAS	n.a.		
^{1}H-RMN	3.455 (3H); 3.495, 3.507, 3.520, 3.532, 3.544 (q, 1H); 3.679, 3.692, 3.705, 3.718 (dd, 2H); 3.734, 3.746, 3.760, 3.772 (dd, 2H); 3.834, 3.893, 3.856, 3.861 (dd, 2H); 3.878, 3.883, 3.900, 3.905 (dd, 2H)		
^{13}C-RMN	58.059; (68.345, 68.682, 69.020, 69.359 (c)); 71.301; 79.042; (119.729, 122.506, 125.285, 128.063 (c))		
^{19}F-RMN	-74.385, -74.362, -74.339		
FT-IR	1162; 1279; 2938		
m/z	270.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	H	O	F	C	H	O	F
35.56	4.48	17.77	42.19	35.4	4.2		42.1

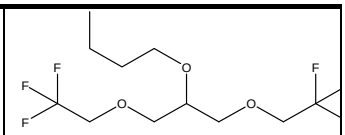
Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.55	μ	4.235	b. p.	178	n_D^{20}	1.3476	log P	1.8322	ν^{20}	1.810

π^*	1.04	**ε**	13.744	**ΔH_{vap}^{eb}**	45.23	**$f_{(dielectric)}$**	0.1762	**H_2O^{sol}**	3.2	**η^{20}**	2.330
α	0.36	**$f_{(kirkwood)}$**	0.4473	**P_{vap}^{298}**	0.429					**ρ^{20}**	1.2871

Name	2-ethoxy-1,3-bis(2,2,2-trifluoroethoxy)propane	**Structure**	
Code	3F,2,3F		
CAS	n.a.		
^{1}H-RMN	1.153, 1.170, 1.188 (t, 3H); 3.573 (m, 1H); 3.590, 3.608 (d, 2H); 3.636, 3.648, 3.662, 3.674 (dd, 2H); 3.688, 3.700, 3.714, 3.726 (dd, 2H); 3.806, 3.813, 3.828, 3.835 (dd, 2H); 3.850, 3.857, 3.872, 3.879 8dd, 2H)		
^{13}C-RMN	15.305; 65.958; (68.320, 68.658, 68.996, 69.33 (c)) 71.692; 77.386; (119.770, 122.547, 125.324, 128.101 (c))		
^{19}F-RMN	-74.423		
FT-IR	1162; 1279; 2882; 2935; 2978		
m/z	284.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
38.04	4.97	16.89	40.11	38.2	4.7		39.0

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.60	**μ**	4.268	**b. p.**	171	**n_D^{20}**	1.3516	**log P**	2.1810	**ν^{20}**	n.a.
π^*	0.91	**ε**	12.81	**ΔH_{vap}^{eb}**	50.08	**$f_{(dielectric)}$**	0.1777	**H_2O^{sol}**	n.a.	**η^{20}**	n.a.
α	0.55	**$f_{(kirkwood)}$**	0.4437	**P_{vap}^{298}**	n.a.					**ρ^{20}**	1.2266

Name	2-*n*-butoxy-1,3-bis(2,2,2-trifluoroethoxy)propane	**Structure**	
Code	3F,4,3F		
CAS	n.a.		
^{1}H-RMN	0.883, 0.901, 0.920 (t, 3H); 1.307, 1.325, 1.343, 1.363, 1.382, 1.400 (m, 2H); 1.502, 1.518, 1.538, 1.555, 1.572 (q, 2H); 3.534, 3.550, 3.567 (t, 2H); 3.554, 3.566, 3.579, 3.592, 3.604 (q, 1H); 3.653, 3.666, 3.678, 3.691, (dd, 2H); 3.703, 3.715, 3.729, 3.741 (dd, 2H); 3.822, 3.830, 3.844, 3.852 (dd, 2H); 3.866, 3.873, 3.888, 3.895 (dd, 2H)		
^{13}C-RMN	13.712; 19.147; 32.000; (68.363, 68.701, 69.039, 69.377, 70.475 (c)); 71.678; 73.044; 77.625; (119.752, 122.531, 125.309, 128.087 (c))		
^{19}F-RMN	-74.401		
FT-IR	1166; 1280; 2876; 2936; 2960		
m/z	312.1		

Theoretical elemental analysis				Experimental elemental analysis			
C	**H**	**O**	**F**	**C**	**H**	**O**	**F**
42.31	5.81	15.37	36.51	42.7	5.7		36.4

Polarity				Vaporization		Polarizability		Hydrophobicity		Others	
E_T^N	0.57	**μ**	n.a.	**b. p.**	208	**n_D^{20}**	n.a.	**log P**	3.1609	**ν^{20}**	n.a.
π^*	1.09	**ε**	n.a.	**ΔH_{vap}^{eb}**	52.77	**$f_{(dielectric)}$**	n.a.	**H_2O^{sol}**	n.a.	**η^{20}**	n.a.
α	0.36	**$f_{(kirkwood)}$**	n.a.	**P_{vap}^{298}**	n.a.					**ρ^{20}**	n.a.