Supplementary Material (ESI) for New Journal of Chemistry

Table S1

Propanone. Data for dry propanone, including solute descriptors

Solute	logKs	Ref	logKw	LogP	E	S	A	B	B	V	L
Helium	-1.45	16	-2.02	0.57	0.000	0.00	0.00	0.00	0.00	0.0680	-1.741
Neon	-1.28	16	-1.96	0.68	0.000	0.00	0.00	0.00	0.00	0.0850	-1.575
Argon	-0.52	16	-1.47	0.95	0.000	0.00	0.00	0.00	0.00	0.1900	-0.688
Krypton	-0.07	17	-1.21	1.14	0.000	0.00	0.00	0.00	0.00	0.2460	-0.211
Xenon	0.50	17	-0.97	1.47	0.000	0.00	0.00	0.00	0.00	0.3290	0.378
Radon	0.75	16	-0.65	1.40	0.000	0.00	0.00	0.00	0.00	0.3840	0.877
Hydrogen	-1.00	16	-1.72	0.72	0.000	0.00	0.00	0.00	0.00	0.1086	-1.200
Oxygen	-0.56	16	-1.51	0.95	0.000	0.00	0.00	0.00	0.00	0.1830	-0.723
Nitrogen	-0.75	16	-1.80	1.05	0.000	0.00	0.00	0.00	0.00	0.2222	-0.978
Nitrous oxide	0.77	16	-0.23	1.00	0.068	0.35	0.00	0.10	0.10	0.2810	0.164
Carbon monoxide	-0.59	16	-1.62	1.03	0.000	0.00	0.00	0.04	0.04	0.2220	-0.836
Carbon dioxide	0.79	16	-0.08	0.87	0.000	0.28	0.05	0.10	0.10	0.2809	0.058
Sulfur dioxide	2.58	17	1.53	1.05	0.370	0.66	0.28	0.10	0.10	0.3465	0.778
Hydrogen sulfide	1.39	17	0.49	0.90	0.310	0.32	0.10	0.08	0.08	0.2721	0.706
Methane	-0.22	16	-1.46	1.24	0.000	0.00	0.00	0.00	0.00	0.2495	-0.323
Ethane	0.50	16	-1.34	1.84	0.000	0.00	0.00	0.00	0.00	0.3904	0.492
Propane	1.00	18	-1.44	2.44	0.000	0.00	0.00	0.00	0.00	0.5313	1.050
Butane	1.56	19	-1.50	3.08	0.000	0.00	0.00	0.00	0.00	0.6722	1.615
Isobutane	1.37	20	-1.70	3.07	0.000	0.00	0.00	0.00	0.00	0.6722	1.409
Pentane	1.98	21	-1.70	3.68	0.000	0.00	0.00	0.00	0.00	0.8131	2.162
2,2-Dimethylpropane	1.63	22	-1.84	3.47	0.000	0.00	0.00	0.00	0.00	0.8131	1.820
Hexane	2.37	21	-1.82	4.22	0.000	0.00	0.00	0.00	0.00	0.9540	2.668
Heptane	2.81	21	-1.96	4.80	0.000	0.00	0.00	0.00	0.00	1.0949	3.173
Octane	3.23	21	-2.11	5.32	0.000	0.00	0.00	0.00	0.00	1.2358	3.677
Nonane	3.66	21	-2.15	5.81	0.000	0.00	0.00	0.00	0.00	1.3767	4.182
2-Methylpentane	2.24	21	-1.84	4.08	0.000	0.00	0.00	0.00	0.00	0.9540	2.503
2,4-Dimethylpentane	2.52	21	-2.08	4.60	0.000	0.00	0.00	0.00	0.00	1.0949	2.809
2,5-Dimethylhexane	2.95	21	-2.02	4.97	0.000	0.00	0.00	0.00	0.00	1.2358	3.308
2,3,4-Trimethylpentane	3.03	21	-1.88	4.91	0.000	0.00	0.00	0.00	0.00	1.2358	3.481
Cyclohexane	2.60	21	-0.90	3.56	0.305	0.10	0.00	0.00	0.00	0.8454	2.964
Methylcyclohexane	2.88	23	-1.21	4.13	0.244	0.06	0.00	0.00	0.00	0.9863	3.319
Ethylcyclohexane	3.32	21	-1.58	4.90	0.263	0.10	0.00	0.00	0.00	1.1272	3.877
Ethene	0.56	16	-0.94	1.50	0.107	0.10	0.00	0.07	0.07	0.3474	0.289
Isobutene	1.74	20	-0.86	2.60	0.120	0.08	0.00	0.08	0.08	0.6292	1.579
trans-But-2-ene	1.81	24	-0.98	2.85	0.126	0.08	0.00	0.05	0.05	0.6292	1.664
1,3-Butadiene	2.01	24	-0.45	2.46	0.320	0.23	0.00	0.10	0.10	0.5862	1.543
Ethyne	1.34	25	0.00	1.34	0.190	0.47	0.12	0.05	0.05	0.3044	0.070
Propyne	1.82	25	0.35	1.47	0.183	0.25	0.12	0.14	0.14	0.4453	1.025
But-1-yne	2.19	25	0.12	2.20	0.178	0.25	0.12	0.10	0.10	0.5862	1.520
Vinylacetylene	2.34	25	-0.03	2.37	0.327	0.26	0.18	0.01	0.01	0.5432	1.467
Chloromethane	1.85	26	0.40	1.45	0.249	0.43	0.00	0.08	0.08	0.3719	1.163
Dichloromethane	3.03	27	0.96	2.07	0.387	0.57	0.10	0.05	0.05	0.4943	2.019

Trichloromethane	3.41	28	0.79	2.62	0.425	0.49	0.15	0.02	0.02	0.6167	2.480
Tetrachloromethane	3.04	28	-0.06	3.10	0.458	0.38	0.00	0.00	0.00	0.7391	2.823
1,1,1-Trichloroethane	3.10	29	0.14	2.96	0.369	0.41	0.00	0.09	0.09	0.7576	2.733
1,1,2,2-Tetrachloroethane	4.60	30	1.81	2.79	0.595	0.76	0.16	0.12	0.12	0.8800	3.803
1,3-Dichloropropane	4.13	29	1.39	2.74	0.408	0.80	0.05	0.12	0.12	0.7761	3.106
1-Chlorobutane	3.12	31	0.12	3.00	0.210	0.40	0.00	0.10	0.10	0.7946	2.722
t-Butyl chloride	2.54	32	-0.80	3.34	0.142	0.30	0.00	0.03	0.03	0.7946	2.273
1,4-Dichlorobutane	4.81	30	1.70	3.11	0.413	0.95	0.00	0.17	0.17	0.9170	3.501
1-Chloropentane	3.56	29	0.05	3.51	0.208	0.38	0.00	0.09	0.09	0.9355	3.223
t-Butyl bromide	2.83	32	-0.62	3.45	0.305	0.29	0.00	0.07	0.07	0.8472	2.609
Iodomethane	2.60	33	0.65	1.95	0.676	0.43	0.00	0.12	0.12	0.5077	2.106
Iodoethane	2.92	34	0.54	2.38	0.640	0.40	0.00	0.14	0.14	0.6486	2.573
$CF_2Cl.CFCl_2$	2.43	35	-1.30	3.73	0.010	0.13	0.00	0.00	0.00	0.8107	2.210
$CFCl_2.CFCl_2$	3.26	36	-0.64	3.90	0.227	0.33	0.00	0.02	0.02	0.9154	3.034
Halothane	3.50	37	0.12	3.42	0.102	0.39	0.13	0.05	0.05	0.7409	1.982
Diethyl ether	2.38	38	1.17	1.21	0.041	0.25	0.00	0.45	0.45	0.7309	2.015
Tetrahydrofuran	3.02	39	2.55	0.47	0.289	0.52	0.00	0.48	0.48	0.6223	2.636
Dioxane	3.72	40	3.71	0.01	0.329	0.75	0.00	0.64	0.64	0.6810	2.892
Propanone	3.04	(a)	2.83	0.25	0.179	0.70	0.04	0.49	0.49	0.5470	1.696
Butanone	3.42	28	2.72	0.70	0.166	0.70	0.00	0.51	0.51	0.6879	2.287
Methyl acetate	3.02	41	2.30	0.72	0.142	0.64	0.00	0.45	0.45	0.6057	1.911
Acetonitrile	2.81	38	2.85	-0.04	0.237	0.90	0.07	0.32	0.32	0.4042	1.739
Ammonia	1.48	42	3.19	-1.67	0.139	0.39	0.16	0.56	0.56	0.2084	0.319
Diethylamine	2.75	43	2.99	-0.24	0.154	0.30	0.08	0.69	0.69	0.7720	2.395
Trimethylamine	1.88	26	2.35	-0.47	0.140	0.20	0.00	0.67	0.67	0.6311	1.620
Triethylamine	2.97	34	2.36	0.61	0.101	0.15	0.00	0.79	0.79	1.0538	3.040
Nitromethane	3.88	40	2.95	0.93	0.313	0.95	0.06	0.31	0.31	0.4237	1.892
N-Methylformamide	5.39	44	6.30	-0.91	0.405	1.30	0.40	0.55	0.55	0.5059	2.687
Dimethylformamide	4.71	45	5.73	-1.02	0.367	1.31	0.00	0.74	0.74	0.6468	3.173
Methanol	3.03	46	3.74	-0.71	0.278	0.44	0.43	0.47	0.47	0.3082	0.970
Ethanol	3.24	28	3.67	-0.43	0.246	0.42	0.37	0.48	0.48	0.4491	1.485
Cyclopentanol	4.60	47	4.03	0.57	0.427	0.54	0.32	0.56	0.56	0.7630	3.241
Cyclohexanol	5.09	47	4.01	1.08	0.460	0.54	0.32	0.57	0.57	0.9040	3.758
SF6	0.05	17	-2.23	2.28	-0.600	-0.20	0.00	0.00	0.00	0.4643	-0.120
Carbon disulfide	2.25	28	-0.15	2.40	0.876	0.26	0.00	0.03	0.03	0.4905	2.370
Tetraethylsilicon	3.84	48	-2.03	5.85	0.126	-0.12	0.00	0.00	0.00	1.4815	4.348
Tetramethyltin	2.55	48	-1.53	4.08	0.324	0.11	0.00	0.10	0.10	1.0431	2.651
Tetraethyltin	4.52	48	-1.62	6.14	0.464	0.18	0.00	0.13	0.13	1.6067	4.923
Tetraethyllead	4.56	48	-1.89	6.45	0.864	0.08	0.00	0.11	0.11	1.6476	5.386
Benzene	3.21	46	0.63	2.58	0.610	0.52	0.00	0.14	0.14	0.7164	2.786
Toluene	3.65	28, 40	0.65	3.00	0.601	0.52	0.00	0.14	0.14	0.8573	3.325
Isopropylbenzene	4.32	49	0.22	4.10	0.602	0.49	0.00	0.16	0.16	1.1391	4.084
Isopropenylbenzene	4.67	49	0.91	3.76	0.851	0.64	0.00	0.19	0.19	1.0961	4.292
Chlorobenzene	4.14	49	0.82	3.32	0.718	0.65	0.00	0.07	0.07	0.8388	3.657
Aniline	5.75	50	4.30	1.45	0.955	0.96	0.26	0.41	0.50	0.8162	3.934
Pyridine	3.97	51	3.44	0.53	0.631	0.84	0.00	0.52	0.47	0.6753	3.022
4-Nitrobenzyl chloride	7.34	52	3.77	3.57	1.080	1.35	0.00	0.35	0.35	1.1539	5.806
Naphthalene	5.75	S2	1.73	4.02	1.340	0.92	0.00	0.20	0.20	1.0854	5.161

Anthracene	8.22	S2	3.03	5.19	2.290	1.34	0.00	0.28	0.28	1.4544	7.568
Phenanthrene	8.26	S2	2.80	5.46	2.055	1.29	0.00	0.29	0.29	1.4544	7.632
Pyrene	9.32	S2	3.50	5.82	2.808	1.71	0.00	0.28	0.28	1.5846	8.833
Tricosane	9.84	S2	-3.72	13.56	0.000	0.00	0.00	0.00	0.00	3.3493	11.252
2-Hydroxybenzoic acid	7.68	S2	5.39	2.29	0.900	0.85	0.73	0.37	0.37	0.9904	4.732
4-Hydroxybenzoic acid	8.44	S2	6.78	1.66	0.930	0.90	0.81	0.56	0.56	0.9904	4.867
Methyl 4-hydroxybenzoate	9.03	S2	6.84	2.19	0.900	1.37	0.69	0.45	0.45	1.1313	5.665
Benzoic acid	7.06	S2	5.10	1.96	0.730	0.90	0.59	0.40	0.40	0.9317	4.657
Salicylamide	9.55	S2	7.60	1.95	1.160	1.58	0.61	0.51	0.51	1.0315	5.818
Acetylsalicylic acid	10.30	S2	8.57	1.73	0.781	1.69	0.71	0.67	0.67	1.2879	6.279
Betulin	20.42	S2	10.39	10.03	1.790	2.12	0.70	1.14	1.14	3.8670	17.470
3-Nitrophthalic acid	13.54	S2	12.67	0.88	1.360	2.01	1.20	0.89	0.89	1.3212	7.780
Adipic acid	9.59	S2	9.43	0.16	0.350	1.21	1.13	0.76	0.76	1.1028	4.457
Flurbiprofen	11.83	S2	7.95	3.98	1.440	1.45	0.62	0.76	0.76	1.8389	8.975
Benzil	9.16	S2	4.87	4.29	1.445	1.59	0.00	0.62	0.62	1.6374	7.611
Ferrocene	5.89	S2	1.92	3.97	1.350	0.85	0.00	0.20	0.20	1.1209	5.622
2-Chlorobenzoic acid	7.60	S2	5.50	2.10	0.840	1.01	0.68	0.40	0.40	1.0541	4.840
4-Chlorobenzoic acid	7.23	S2	4.80	2.43	0.840	1.02	0.63	0.27	0.27	1.0541	4.947

[a] defined as unity.

Table S2

Propanone. Data on solubilities in dry propanone and water

	logSs	logSw	logP	logKw	logKs	Ref
Naphthalene	0.44	-3.58	4.02	1.73	5.75	53
Anthracene	-1.24	-6.43	5.19	3.03	8.22	54
Phenanthrene	0.29	-5.17	5.46	2.80	8.26	54
Pyrene	-0.33	-6.15	5.82	3.50	9.32	55
Tricosane	-1.81	-15.37	13.56	-3.72	9.84	56
2-Hydroxybenzoic acid	0.37	-1.92	2.29	5.39	7.68	57
4-Hydroxybenzoic acid	0.19	-1.47	1.66	6.78	8.44	58
Methyl 4-hydroxybenzoate	0.36	-1.83	2.19	6.84	9.03	59
Benzoic acid	0.37	-1.59	1.96	5.10	7.06	58
Salicylamide	0.20	-1.75	1.95	7.60	9.55	60
Acetylsalicylic acid	0.05	-1.68	1.73	8.57	10.30	61
Betulin	-1.67	-11.70	10.03	10.39	20.42	62
3-Nitrophthalic acid	-0.15	-1.03	0.88	12.67	13.54	63
Adipic acid	-0.66	-0.82	0.16	9.43	9.59	64
Flurbiprofen	0.14	-3.74	3.88	7.95	11.83	65
Benzil	0.24	-4.05	4.29	4.87	9.16	65
Ferrocene	-0.50	-4.47	3.97	1.92	5.89	66
2-Chlorobenzoic acid	0.20	-1.89	2.10	5.50	7.60	65
4-Chlorobenzoic acid	-0.86	-3.29	2.43	4.80	7.23	65

Table S3.
Butanone. Data for dry butanone

Solute	logKs	Ref	logKw	LogP
Hydrogen	-1.06	73	-1.72	0.66
Nitrogen	-0.79	73	-1.80	1.01
Nitrous oxide	0.69	73	-0.23	0.92
Oxygen	-0.56	18	-1.51	0.95
Carbon dioxide	0.72	73	-0.08	0.80
Ammonia	1.42	74	3.19	-1.77
Butane	1.69	19	-1.52	3.21
Pentane	2.07	21	-1.70	3.77
Hexane	2.52	21	-1.82	4.34
2-Methylpentane	2.39	21	-1.84	4.23
Heptane	3.03	21	-1.96	4.99
2,4-Dimethylpentane	2.68	21	-2.08	4.76
Octane	3.45	21	-2.11	5.56
2,5-Dimethylhexane	3.14	21	-2.02	5.16
2,2,4-Trimethylpentane	2.97	75	-2.12	5.09
2,3,4-Trimethylpentane	3.22	21	-1.88	5.10
Nonane	3.90	21	-2.15	6.05
Decane	4.42	76	-2.32	6.74
Cyclohexane	2.75	21	-0.90	3.65
Methylcyclohexane	3.02	34	-1.21	4.23
Ethylcyclohexane	3.53	21	-1.58	5.11
Propene	1.13	77	-0.97	2.10
Isoprene	2.40	78	-0.50	2.90
Pent-1-ene	2.11	78	-1.23	3.34
Isopentene	1.99	78	-1.34	3.33
2,4,4-Trimethylpent-1-ene	3.18	75	-1.47	4.65
2,4,4-Trimethylpent-2-ene	3.22	75	-1.35	4.57
Cyclohexene	2.93	79	-0.27	3.20
Cyclohexa-1,4-diene	3.23	79	0.59	2.64
Dichloromethane	2.97	78	0.96	2.01
Trichloromethane	3.46	80, 81	0.79	2.67
Tetrachloromethane	3.04	75	-0.19	3.23
1-Chloropropane	2.70	78	0.24	2.46
2-Methyl-2-chloropropane	2.68	78	-0.80	3.48
1,2-Dichloroethane	3.51	34	1.31	2.20
Bromoethane	2.59	78, 34	0.54	2.05
Iodomethane	2.55	78	0.65	1.90
Iodoethane	2.98	78	0.54	2.44
1,1,2-Trichlorotrifluoroethane	2.46	35	-1.30	3.76
Tetrachloroethene	3.65	74	-0.07	3.72
Dipropyl ether	3.20	82	0.85	2.35

Diisopropyl ether	2.86	82	1.17	1.69
1,4-Dioxane	3.68	40	3.71	-0.03
Ethyl formate	2.72	83	1.96	0.76
Ethyl acetate	3.29	34	2.16	1.13
Proprionaldehyde	2.82	84	2.52	0.30
Propanone	2.92	85, 86	2.83	0.09
Butanone	3.36	78	2.72	0.64
Nitromethane	3.65	34	2.95	0.70
Nitromethane	3.85	85	2.95	0.90
Acetonitrile	3.27	34, 87	2.85	0.42
Triethylamine	3.05	88	2.36	0.69
N,N-Dimethylformamide	4.70	89	5.73	-1.03
Methanol	2.81	34	3.74	-0.93
Ethanol	3.17	40	3.67	-0.50
Propan-1-ol	3.64	90	3.56	0.08
Propan-2-ol	3.33	90	3.48	-0.15
Butan-1-ol	4.15	90	3.46	0.69
Butan-2-ol	3.80	91	3.39	0.41
2-Methylpropan-1-ol	3.98	91	3.30	0.68
2-Methylpropan-2-ol	3.45	91	3.28	0.17
Hexan-1-ol	5.10	90	3.23	1.87
Octan-1-ol	6.01	90	3.00	3.01
Acetic acid	3.97	92	4.88	-0.91
Benzene	3.29	76	0.63	2.66
Toluene	3.74	40	0.65	3.09
Ethylbenzene	4.14	92	0.58	3.56
Carbon disulfide	2.27	78	-0.15	2.42
Pyridine	3.94	93	3.44	0.50
Eicosane	9.25	S4	-3.31	12.56
Docosane	9.96	S4	-3.57	13.53
Tricosane	10.51	S4	-3.72	14.23
Tetracosane	10.82	S4	-3.84	14.66
Octacosane	12.52	S4	-4.34	16.86
Tetradecanol	9.23	S4	2.26	6.97
Hexadecanol	10.13	S4	2.02	8.11
Octadecanol	10.08	S4	1.78	8.30
Anthracene	8.32	S4	3.03	5.29
Phenanthrene	8.27	S4	2.80	5.47
Pyrene	9.50	S4	3.50	6.00
trans-Stilbene	8.40	S4	2.78	5.62
Benzil	9.15	S4	4.87	4.28
2-Hydroxybenzoic acid	7.62	S4	5.39	2.23

Table S4

Butanone. Data on solubilities in dry butanone and in water

Solute	logSw	logSs	logP	logKw	logKs	Ref
Eicosane	-12.99	-0.414	12.56	-3.31	9.25	94
Docosane	-14.53	-1.001	13.53	-3.57	9.96	94
Tricosane	-15.37	-1.144	14.23	-3.72	10.51	94, 95
Tetracosane	-16.14	-1.478	14.66	-3.84	10.82	94
Octacosane	-19.30	-2.441	16.86	-4.34	12.52	94, 95
Tetradecanol	-6.01	0.415	6.97	2.26	9.23	96
Hexadecanol	-7.20	-0.087	8.11	2.02	10.13	96
Octadecanol	-8.39	-0.642	8.30	1.78	10.08	96
Anthracene	-6.43	-1.139	5.29	3.03	8.32	57
Phenanthrene	-5.17	0.303	5.47	2.80	8.27	97
Pyrene	-6.15	-0.151	6.00	3.50	9.50	97
trans-Stilbene	-5.80	-0.183	5.62	2.78	8.40	57
Benzil	-4.05	0.234	4.28	4.87	9.15	98
2-Hydroxybenzoic acid	-1.92	0.308	2.23	5.39	7.62	99

Table S5

Butanone.

Data for wet butanone taken from ref. 12

Solute	logKs	logKw	logP
Formaldehyde	1.30	2.02	-0.72
Formic acid	5.46	5.33	0.13
Acetic acid	4.96	4.88	0.08
Propanoic acid	5.15	4.73	0.42
Butanoic acid	5.35	4.63	0.72
Pentanoic acid	5.46	4.45	1.01
Hexanoic acid	5.67	4.31	1.36
Dipterex	8.64	8.56	0.08
O,O-Dimethyl dichlorovinyl phosphonate	5.76	5.04	0.72
Methylphosphonic acid, dimethyl ester	4.66	5.39	-0.73
Maleic acid	8.83	8.30	0.53
Citric acid	10.34	10.82	-0.48
Succinic acid	9.23	9.23	0.00
Adipic acid	9.73	9.43	0.30
Suberic acid	10.61	9.93	0.68
Hydrogen peroxide	5.53	5.69	-0.16

Supplementary Material (ESI) for New Journal of Chemistry

Table S6
Cyclohexanone. Data for dry cyclohexanone

	LogKs	LogKw	LogP	Ref
Helium	-1.804	-2.02	0.216	100
Neon	-1.654	-1.96	0.306	100
Argon	-0.767	-1.47	0.703	100
Krypton	-0.274	-1.21	0.936	100
Xenon	0.356	-0.97	1.326	100
Hydrogen	-1.286	-1.72	0.434	100
Deuterium	-1.266	-1.73	0.464	100
Nitrogen	-1.054	-1.80	0.746	100
Oxygen	-0.828	-1.51	0.682	100
Sulfur hexafluoride	-0.379	-2.22	1.841	100
Carbon dioxide	0.576	-0.08	0.656	100
Ethane	0.387	-1.34	1.727	100
Pentane	1.977	-1.70	3.677	21
2-Methylbutane	1.892	-1.75	3.642	101
Hexane	2.439	-1.82	4.259	21
2-Methylpentane	2.303	-1.84	4.143	21
Heptane	2.947	-1.96	4.907	101
2,4-Dimethylpentane	2.596	-2.08	4.676	21
Octane	3.419	-2.11	5.529	40
2,5-Dimethylhexane	3.063	-2.02	5.083	21
2,3,4-Trimethylpentane	3.152	-1.88	5.032	21
Nonane	3.846	-2.15	5.996	21
Cyclohexane	2.812	-0.90	3.712	101
Ethylcyclohexane	3.548	-1.58	5.128	21
Ethene	0.401	-0.94	1.341	100
Pent-1-ene	2.028	-1.23	3.258	78
Isopentene (3-methylbut-1-ene)	1.912	-1.34	3.252	78
2-Methylbut-2-ene	2.264	-0.96	3.224	101
Isoprene	2.342	-0.50	2.842	78
Tetrafluoromethane	-1.031	-2.29	1.259	100
Dichloromethane	3.024	0.96	2.064	78
Trichloromethane	3.468	0.79	2.678	78
Tetrachloromethane	3.167	-0.19	3.357	101
1-Chloropropane	2.689	0.24	2.449	78
tert-Butyl chloride	2.666	-0.80	3.466	78
Bromoethane	2.601	0.54	2.061	78
Iodomethane	2.624	0.65	1.974	78
Iodoethane	3.066	0.54	2.526	78
1,4-Dioxane	3.666	3.71	-0.044	40

Propanone	2.789	2.83	-0.041	78
Butanone	3.294	2.72	0.574	40
Cyclohexanone	4.651	3.60	1.051	(a)
Ethyl acetate	3.177	2.16	1.017	78
Ethanol	3.162	3.67	-0.508	40
Nitromethane	3.711	2.95	0.761	40
Benzene	3.297	0.63	2.667	101
Toluene	3.794	0.65	3.144	40
Carbon disulfide	2.424	-0.15	2.574	78
Acetonitrile	3.151	2.85	0.301	78
Triethylamine	3.014	2.36	0.654	78
Glutaric acid	8.850	9.32	-0.470	S6
Adipic acid	9.430	9.43	0.000	S6
Benzil	9.210	4.87	4.340	S6
Fumaric acid	7.260	7.30	-0.040	S6
Succinic acid	8.540	9.23	-0.690	S6
Phenanthrene	8.330	2.80	5.530	S6
Anthracene	8.530	3.03	5.500	S6
Pyrene	9.650	3.50	6.150	S6
Naphthalene	5.660	1.73	3.930	S6
2-Hydroxybenzoic acid	7.660	5.39	2.270	S6
Benzo[ghi]perylene	14.230	6.58	7.650	S6
Temazepam	14.383	11.13	3.253	S6

[a] Activity coefficient defined as unity.

Table S7
Cyclohexanone. Data on solubilities in dry cyclohexanone and in water

	logSw	logSs	logP	logKw	logKs	Ref
Glutaric acid	0.717	0.247	-0.470	9.32	8.850	102
Adipic acid	-0.820	-0.818	0.000	9.43	9.430	103, 104
Benzil	-4.050	0.294	4.340	4.87	9.210	98
Fumaric acid	-1.240	-1.276	-0.040	7.30	7.260	103
Succinic acid	-0.178	-0.866	-0.690	9.23	8.540	103
Phenanthrene	-5.170	0.361	5.530	2.80	8.330	97
Anthracene	-6.430	-0.933	5.500	3.03	8.530	57
Pyrene	-6.150	-0.004	6.150	3.50	9.650	57
Naphthalene	-3.580	0.349	3.930	1.73	5.660	105
2-Hydroxybenzoic acid	-1.920	0.352	2.270	5.39	7.660	99
Benzo[ghi]perylene	-9.020	-1.371	7.650	6.58	14.230	106
Temazepam	-3.474	-0.221	3.253	11.13	14.383	107

Table S8
Methyl isobutyl ketone (MIBK).Data for wet MIBK taken from ref 12.

Solute	logP	logKw	logKs
Methacrylic acid	1.08	4.46	5.54
4-Acetyl-1-phenyl-3-methyl-5-pyrazolone	1.77	7.25	9.02
Acetylacetone	0.80	3.54	4.34
Aceticacid, acetylamino	-1.50	10.73	9.23
6-Isopropyltropalone	2.40	5.37	7.77
Acetic acid	-0.27	4.88	4.61
Lactic acid	-0.80	7.05	6.25
5-Pyrazolone,1-phenyl-3-methyl-4-benzoyl	2.93	8.48	11.41
Sorbic acid	1.10	5.15	6.25
4-Propionyl-1-phenyl-3-methyl-5-pyrazolone	2.38	7.14	9.52
Propionic acid	0.34	4.73	5.07
4-Butyryl-1-phenyl-3-methyl-5-pyrazolone	2.91	6.97	9.88
Butyric acid	0.79	4.63	5.42
4-Hexanoyl-1-phenyl-3-methyl-5-pyrazolone	4.18	6.79	10.97
4-Octanoyl-1-phenyl-3-methyl-5-pyrazolone	5.36	6.49	11.85
Octanoic acid	3.06	4.15	7.21
4-Decanoyl-1-phenyl-3-methyl-5-pyrazolone	6.62	6.28	12.90
Dioctylphosphate	5.82	6.76	12.58
Dibutylphosphate	1.36	7.89	9.25
Dibutylphosphorodithiotic acid	2.54	5.89	8.43
Triethylamine	0.61	2.36	2.97
Diethylamine	-0.32	2.99	2.67
Ethanol	-0.40	3.67	3.27
Diethylphosphate	-0.56	9.07	8.51
Methylamine	-0.31	3.34	3.03
Trimethylamine	-0.27	2.35	2.08
Dimethylamine	-0.92	3.15	2.23
Ephedrine	0.71	6.88	7.59
Methoxyacetic acid	-0.57	5.71	5.14
3,5-Dimethylphenol	2.91	4.60	7.51
m-Cresol	2.42	4.60	7.02
8-Quinolinol,4-methyl	2.63	3.96	6.59
8-Quinolinol,2-methyl	2.50	4.06	6.56
Diantipyrylmethane	0.38	17.29	17.67
1,1,1-Trifluoro-4(2-thienyl)-4-mercaptobut-3-en-2-one	4.00	3.16	7.16

Thenoyltrifluoroacetone	2.20	4.51	6.71
Ammonia	-1.30	3.19	1.89
Cyanamide	-0.23	4.93	4.70
Aniline	1.50	4.30	5.80
Furfural	1.32	3.83	5.15
1H-1,2,4-Triazole,3-nitro	0.28	7.04	7.32
Succinic acid	-0.69	9.23	8.54
Acrylic acid	0.40	4.55	4.95
Maleic acid	-0.66	8.30	7.64
Cinnamic acid	2.33	6.17	8.50
Aconitic acid	-0.26	12.85	12.59
Propanetricarboxylic acid	-1.00	13.18	12.18
Malonic acid	-0.73	9.00	8.27
β-Carboxyadipic acid	-0.83	14.43	13.60
Succinic acid	-0.71	9.23	8.52
Glutaric acid	-0.45	9.32	8.87
Adipic acid	-0.10	9.43	9.33
Suberic acid	0.68	9.93	10.61
Diglycolic acid	-1.27	10.35	9.08
Phenoxyaceticacid, p-hydroxy	1.05	11.55	12.60
Phenoxyaceticacid, m-chloro	2.32	7.18	9.50
Phenoxyaceticacid, m-nitro	1.88	9.07	10.95
Phenoxyacetic acid	1.54	7.31	8.85
Benzoicacid, 3,5-dinitro	2.48	8.30	10.78
Sulfosalicylic acid	-1.25	14.04	12.79
2,4-Dihydroxybenzoic acid	1.55	8.39	9.94
o-Phthalic acid	0.44	11.89	12.33
Salicylic acid	2.51	5.39	7.90
Tartaric acid	-1.58	11.85	10.27
Malic acid	-1.36	11.33	9.97
Formic acid	-0.33	5.33	5.00
Benzoylphenylhydroxylamine	2.25	7.90	10.15
Hydrogen peroxide	-0.90	5.69	4.79
Dibenzylphosphoric acid	1.81	12.46	14.27
Phosphoricacid, bis(p-chlorophenyl)ester	2.05	11.33	13.38
2-Nitroso-1-naphthol	2.30	6.44	8.74
Citric acid	-1.62	10.82	9.20
1,3,5-Trihydroxybenzene	0.59	11.42	12.01
1,2,4-Trihydroxybenzene	0.70	11.02	11.72

1,4-Dihydroxybenzene	1.00	8.87	9.87
1,3-Dihydroxybenzene	1.22	8.35	9.57
1,2,3-Trihydroxybenzene	0.55	10.36	10.91
1-Naphthol	3.63	5.87	9.50
8-Quinolinol	2.13	4.44	6.57
Phenol	2.02	4.85	6.87
2-Chlorophenol	2.69	3.34	6.03
Catechol	1.29	7.20	8.49
1-Nitroso-2-naphthol	2.60	5.36	7.96
Pyridine	0.46	3.44	3.90
Naphthalene	3.71	1.73	5.44
8-Quinolinol	1.80	4.44	6.24
Erythromycin	1.16		
Berythromycin	1.30		