

Supplementary Information

Table1 Motivating example. Data for five properties and seven hypothetical solvents.

Solvents	Vapour Pressure (mbar)	Viscosity (cP)	Surface Tension (dyne/cm)	Acute Toxicity	CO ₂ Solubility (MPa ^{0.5})
A	0.57	9.98	21.69	0.37	36.4
B	1.32	6.37	34.28	0.20	17.4
C	0.77	4.51	27.51	0.12	8.9
D	1.18	5.97	23.26	0.17	23.7
E	0.94	9.33	34.35	0.22	6.3
F	1.08	8.34	28.85	0.28	27.1
G	1.8	7.55	33.66	0.28	32.5

Table2 CAS numbers and Chemical Name of 125 solvents.

	CAS No.	Chemical Name
1	110-18-9	N,N,N',N'-Tetramethylethylenediamine
2	110-96-3	Diisobutylamine
3	626-23-3	Disec-butylamine
4	39099-23-5	N-Isopropylbutylamine
5	20634-92-8	Ethyl-di-N-propyl amine
6	4444-68-2	N,N-diethylbutan-1-amine
7	111-92-2	Di-n-butylamine
8	102-69-2	Tripropylamine
9	2439-54-5	n-Methyloctylamine
10	109-55-7	3-Dimethylaminopropylamine
11	112-20-9	n-Nonylamine, 1-Aminononane
12	111-86-4	n-Octylamine
13	2016-57-1	n-Decylamine
14	111-68-2	n-Heptylamine
15	111-26-2	Hexylamine
16	2050-92-2	Dipentylamine
17	7005-47-2	2-Dimethylamino-2-methylpropanol
18	124-22-1	Dodecylamine, Laurylamine
19	811-93-8	1,2-Propanediamine, 2-methyl-,Nsc17717
20	143-16-8	Diethylamine
21	16369-05-4	DL-2-Amino-3-methyl-1-butanol
22	96-80-0	2-(Diisopropylamino)ethanol
23	102-82-9	Tributylamine
24	1120-24-7	N,N-dimethyldodecan-1-amine
25	3179-63-3	3-Dimethylamino-1-propanol
26	4146-04-7	2-aminopentan-1-ol, 2-azanylpentan-1-ol
27	96-20-8	2-Amino-1-butanol
28	5665-74-7	2-Aminohexan-1-ol
29	108-16-7	1-Dimethylamino-2-propanol

	CAS No.	Chemical Name
30	109-56-8	2-Isopropylaminoethanol
31	4620-70-6	2-(tert-Butylamino)ethanol
32	1120-48-5	Di-n-octylamine
33	621-77-2	Tripropylamine
34	2212-32-0	2-[2-dimethylaminoethyl(methylamino)ethanol
35	622-93-5	3-Diethylamino-1-propanol
36	100-37-8	N,N-Diethylethanolamine
37	13330-96-6	4-(dimethylamino)-1-Butanol
38	16369-21-4	2-(propylamino)ethanol
39	5966-51-8	1,3-Bis(dimethylamino)-2-propanol
40	373-44-4	1,8-Diaminooctane
41	646-19-5	1,7-Diaminoheptane
42	124-09-4	1,6-Hexanediamine
43	462-94-2	1,5-Diaminopentane
44	110-60-1	1,4-Diaminobutane
45	39884-48-5	4-Amino-2-butanol
46	109-76-2	1,3-Diaminopropane
47	78-96-6	DL-1-Amino-2-propanol
48	13532-77-9	5-Amino-2,2-dimethylpentanol
49	4048-33-3	6-Amino-1-hexanol
50	2508-29-4	5-Amino-1-pentanol
51	13325-10-5	4-Amino-1-butanol
52	534-03-2	2-Amino-1,3-propanediol
53	621-56-7	3-(Diethylamino)-1,2-propanediol
54	139-87-7	N-Ethyldiethanolamine
55	102-79-4	N-N-Butyldiethanolamine
56	40137-22-2	3-Methylamino-1,2-propanediol
57	64037-42-9	2-Butanol, 3-methyl-3-(N-methyl-N-isopropyl)amino-, hydrochloride
58	16667-45-1	1-(Methylamino)-2-propanol
59	40898-98-4	1-Amino-2,2-dimethylpropan-1-ol
60	50540-24-4	2-N-Butyl-2-methylpropane-1,2-diamine
61	10171-78-5	3-(2-Aminopropylamino)propan-1-ol
62	7328-91-8	2,2-Dimethyl-1,3-propanediamine
63	590-88-5	Butane-1,3-diamine
64	53369-71-4	N,N,2,2-Tetramethyl-1,3-propanediamine
65	29773-01-1	n,n,2,3,3-pentamethylbutan-2-amine hydrobromide(1:1)
66	97-84-7	N,N,N',N'-TetraMethyl-1,3-diaMinobutane
67	6105-72-2	N,N,2-Trimethylpropane-1,3-diamine
68	372-66-7	6-Amino-2-methyl-2-heptanol
69	25620-58-0	2,2,4(2,4,4)-Trimethyl-1,6-hexanediamine
70	51411-49-5	1-Amino-2-methylbutan-2-ol

	CAS No.	Chemical Name
71	4083-57-2	3-Amino-2,4-dimethylpentane
72	6322-01-6	1-amino-3-(diethylamino)-2-propanol
73	1185-93-9	3-Pentanamine,N-ethyl-3-methyl-, hydrochloride (1:1)
74	63765-79-7	2-amino-2-methylhexan-3-ol
75	68367-53-3	1,2-Bis(dimethylamino)-2-methylpropane
76	84642-65-9	2-((3-(Dimethylamino)-2,2-dimethylpropyl)amino)
77	15673-00-4	3,3-Dimethylbutylamine
78	140-80-7	2-Amino-5-diethylaminopentane
79	68955-53-3	1,2-Bis(dimethylamino)-2-methylpropane
80	17086-16-7	2-Heptanol,2-methyl-6-(methylamino)-, hydrochloride (1:1)
81	5448-29-3	2-amino-1,1-dimethylethylisopropylamine
82	927-55-9	4-Amino-1-pentanol
83	33326-98-6	N,3-diethyl-n-methylpentan-3-amine,hydrobromide
84	26535-68-2	2-[(1-methylheptyl)amino]ethanol
85	63732-18-3	1,2-Butanediamine, 1-(N,N-dimethyl
86	33327-00-3	2-Butylamine, N-ethyl-N,2,3,3-tetramethyl-, hydrobromide
87	7173-57-1	3-Aminopropyl(octyl)amine
88	41999-70-6	2-[(3-aminopropyl)methylamino]ethanol
89	27431-62-5	4-(Diethylamino)butylamine
90	105-04-4	N,N,N'-Triethylethylenediamine
91	78718-56-6	Ethanol,2-[[3-(dimethylamino)propyl](2-methylpropyl)amino]
92	69559-11-1	2-(4-Aminopentyl(ethyl)amino)ethanol
93	13205-56-6	2-Aminoundecane
94	24229-53-6	N2-(2-aminoethyl)-N1,N1-dimethylethylenediamine
95	19764-58-0	N2,N2-dimethylpropane-1,2-diamine
96	68603-41-8	Amides, C10-16, N-(2-hydroxypropyl
97	24552-03-2	3-(Dimethylamino)hexane
98	4271-27-6	N,N-diethyl-1-dodecanamine
99	56684-95-8	2,2'-(methylimino)dipropanol
100	67398-36-1	1,1-Dimethyl-2-pentylhydrazine
101	111-41-1	N-(2-Hydroxyethyl)ethylenediamine
102	111-75-1	2-(Butylamino)ethanol
103	111-42-2	Diethanolamine
104	100-37-8	2-(Diethylamino)ethanol
105	111-40-0	Diethylenetriamine
106	110-97-4	Bis(2-hydroxypropyl)amine
107	108-01-0	2-Dimethylaminoethanol
108	107-15-3	Ethylenediamine

	CAS No.	Chemical Name
109	110-73-6	2-(Ethylamino)ethanol
110	6291-84-5	3-(Methylamino)propylamine
111	105-59-9	N-Methyldiethanolamine
112	141-43-5	Ethanolamine
113	78-90-0	1,2-Diaminopropane
114	109-83-1	2-(Methylamino)ethanol
115	112-57-2	Tetraethylenepentamine
116	102-71-6	Triethanolamine
117	156-87-6	3-Amino-1-propanol
118	122-20-3	Triisopropanolamine
119	6168-72-5	DL-2-Amino-1-propanol
120	124-68-5	2-Amino-2-methyl-1-propanol
121	77-86-1	2-Amino-2-methylol-1,3-propanediol
122	115-69-5	2-Amino-2-methyl-1,3-propanediol
123	115-70-8	2-Amino-2-ethyl-1,3-propanediol
124	623-57-4	3-(Dimethylamino)-1,2-propanediol
125	5467-48-1	4-(Diethylamino)butan-2-ol