

Reparameterization of COSMO-SAC for Phase Equilibrium Properties Based on Critically Evaluated Data

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Table S1. Relative deviations of vapor pressures over liquid binaries at temperature T and mole fraction of the first component x_1 calculated with Model I (Δ_I) and Model II (Δ_{II}) from the experimental values^a

Component 1 ^b		Component 2 ^b		x_1	T / K	Reference code			$100\Delta_I$	$100\Delta_{II}$	
Name	Formula	Name	Formula								
argon	Ar	nitrogen	N2	0.154	78.6	1965	wil	sil	0	9.7	9.6
argon	Ar	oxygen	O2	0.247	89.97	1978	yor	yos	0	0.5	0.4
bromine	Br2	tetrachloromethane	CCl4	0.969	331.02	1950	spi	kru	0	-1.4	-1.4
bromine	Br2	1,1,2-trichloro-1,2,2-trifluoroethane	C2Cl3F3	0.919	319.23	1951	spi	mey	0	-50.7	-50.7
dichlorodifluoromethane	CCl2F2	1,1-difluoroethane	C2H4F2	0.866	233.18	1967	kri		0	-6	-5.8
tetrachloromethane	CCl4	trichloromethane	CHCl3	0.374	313.13	1954	mcg	pru	0	0.3	0.4
tetrachloromethane	CCl4	dichloromethane	CH2Cl2	0.918	303.14	1984	azp	roy	0	3.5	4
tetrachloromethane	CCl4	methanol	CH4O	0.455	328.13	1952	sca	tic	0	-10.5	-10.6
tetrachloromethane	CCl4	methanol	CH4O	0.982	303.14	1968	wol	hoe	0	-19.7	-17.8
tetrachloromethane	CCl4	tetrachloroethene	C2Cl4	0.488	343.13	1969	fri	fra	0	-0.8	-0.8
tetrachloromethane	CCl4	1,1,2,2-tetrachloroethane	C2H2Cl4	0.236	298.15	2005	gar	per	0	-2.3	-2.1
tetrachloromethane	CCl4	1,1,1-trichloroethane	C2H3Cl3	0.701	298.14	1976	mei	bro	0	-2.2	-2.1
tetrachloromethane	CCl4	acetonitrile	C2H3N	0.191	318.13	1954	bro	smi	1	0.2	1.4
tetrachloromethane	CCl4	1,2-dibromoethane	C2H4Br2	0.788	303.15	1994	per	val	0	1.5	1.7
tetrachloromethane	CCl4	1,2-dichloroethane	C2H4Cl2	0.503	313.15	1990	emb	ber	0	12.2	12.9
tetrachloromethane	CCl4	ethanoic acid	C2H4O2	0.797	313.14	1969	mik	rat	0	15	14.8
tetrachloromethane	CCl4	ethanol	C2H6O	0.767	327.53	1904	sch		0	-10.5	-10
tetrachloromethane	CCl4	ethanol	C2H6O	0.364	332.53	1969	bou	enj	0	-12	-11.7
tetrachloromethane	CCl4	1,3-dichloropropane	C3H6Cl2	0.858	303.14	1984	azi	roy	0	-5.4	-5.2
tetrachloromethane	CCl4	acetone	C3H6O	0.032	304.33	1952	bac	sim	0	-1.1	-1
tetrachloromethane	CCl4	ethyl methanoate	C3H6O2	0.332	318.14	1983	oht	kin	0	3.2	3.4
tetrachloromethane	CCl4	propanoic acid	C3H6O2	0.376	323.14	1971	lis		1	36.9	36.4
tetrachloromethane	CCl4	propanoic acid	C3H6O2	0.26	363.13	1976	pau		0	13.7	13
tetrachloromethane	CCl4	dimethylformamide	C3H7NO	0.36	303.13	1966	qui		1	-17.7	-16.6
tetrachloromethane	CCl4	2-propanol	C3H8O	0.462	342.55	1963	yua	lu	0	-8.7	-8

tetrachloromethane	CCl4	1-propanol	C3H8O	0.974	348.24	1973	oco	toj	0	-0.4	0.4
tetrachloromethane	CCl4	furan	C4H4O	0.555	303.14	1973	bye	gib	0	11.9	12.4
tetrachloromethane	CCl4	1,4-dioxane	C4H8O2	0.122	298.14	1972	des	osw	0	1.7	2.1
tetrachloromethane	CCl4	ethyl ethanoate	C4H8O2	0.398	323.12	1900	von		0	4.2	4.5
tetrachloromethane	CCl4	ethyl ethanoate	C4H8O2	0.603	303.13	1966	ste	bit	0	3	3.3
tetrachloromethane	CCl4	1-butanol	C4H10O	0.223	346.13	1983	lin		1	-16	-14.9
tetrachloromethane	CCl4	2-methyl-2-propanol	C4H10O	0.886	298.14	1968	bru	del	0	-5.1	-4.6
tetrachloromethane	CCl4	(RS)-2-butanol	C4H10O	0.977	346.13	1983	lin		0	-0.7	-0.1
tetrachloromethane	CCl4	cyclopentane	C5H10	0.483	298.14	1969	bou	lam	0	-0.5	-0.5
tetrachloromethane	CCl4	benzene	C6H6	0.852	312.13	1904	sch		0	3.1	3.3
tetrachloromethane	CCl4	benzene	C6H6	0.493	303.13	1938	tah		0	4.2	4.7
tetrachloromethane	CCl4	benzene	C6H6	0.224	293.14	1963	ste	bit	0	2.8	3.2
tetrachloromethane	CCl4	benzene	C6H6	0.836	311.84	1975	men	con	0	2.5	2.8
tetrachloromethane	CCl4	phenol	C6H6O	0.9	298.14	1961	del		1	-0.9	-0.3
tetrachloromethane	CCl4	aniline	C6H7N	0.458	318.13	1967	des	pan	0	8.9	5.9
tetrachloromethane	CCl4	cyclohexane	C6H12	0.562	333.12	1963	dvo	bou	0	-1.2	-1.2
tetrachloromethane	CCl4	1-hexene	C6H12	0.75	345.03	1969	rod	hsu	0	-3.3	-3.2
tetrachloromethane	CCl4	methylcyclopentane	C6H12	0.358	346.03	1969	rod	hsu	0	-0.7	-0.8
tetrachloromethane	CCl4	toluene	C7H8	0.7	348.12	1926	sch		0	2.4	2.6
tetrachloromethane	CCl4	toluene	C7H8	0.196	313.15	1993	gor	zaw	0	3.6	4
tetrachloromethane	CCl4	methoxybenzene	C7H8O	0.75	288.14	1924	wei	sch	2	-0.4	-0.1
tetrachloromethane	CCl4	3-methylphenol	C7H8O	0.684	293.14	1956	bru	bon	0	-2.2	-1.3
tetrachloromethane	CCl4	octane	C8H18	0.504	308.14	1971	jai	gup	0	-4.2	-4.2
trichloromethane	CHCl3	methanol	CH4O	0.196	330.92	1962	nag		4	-15.6	-15.3
trichloromethane	CHCl3	methanol	CH4O	0.152	303.15	1990	gor	ora	0	-17.2	-17.3
trichloromethane	CHCl3	carbon disulfide	CS2	0.8	283.09	1926	sch		0	-5.9	-6.2
trichloromethane	CHCl3	ethanol	C2H6O	0.301	308.11	1938	sca	ray	0	-28.5	-27.2
trichloromethane	CHCl3	ethanol	C2H6O	0.624	323.14	1975	abb	van	0	-12.9	-11.1
trichloromethane	CHCl3	ethanol	C2H6O	0.363	333.15	1995	fu	mo	0	-19.4	-17.8
trichloromethane	CHCl3	acetone	C3H6O	0.493	308.3	1900	von		0	-5.1	-6.2
trichloromethane	CHCl3	acetone	C3H6O	0.9	273.15	1921	sch		1	-3.4	-3.6

trichloromethane	CHCl3	acetone	C3H6O	0.447	332.72	1949	for	sim	0	-20.5	-21.6
trichloromethane	CHCl3	acetone	C3H6O	0.05	298.14	1960	rab	nik	0	-0.2	-0.3
trichloromethane	CHCl3	acetone	C3H6O	0.784	298.14	1981	tam	ape	1	-2.6	-3.3
trichloromethane	CHCl3	ethyl methanoate	C3H6O2	0.378	318.14	1980	oht	asa	0	-4.6	-5.1
trichloromethane	CHCl3	1,3-dioxacyclopentane	C3H6O2	0.39	323.14	1989	wu	san	0	-11.2	-11.9
trichloromethane	CHCl3	1-propanol	C3H8O	0.496	342.05	1994	wan	cai	1	-11.8	-9.5
trichloromethane	CHCl3	2-thiabutane	C3H8S	0.74	336.02	1958	mat	kra	0	-1.1	-1.5
trichloromethane	CHCl3	butanone	C4H8O	0.928	318.14	1980	oht	asa	0	1.3	1.2
trichloromethane	CHCl3	ethyl ethanoate	C4H8O2	0.305	313.14	1980	oht	asa	0	-1.2	-2
trichloromethane	CHCl3	diethyl ether	C4H10O	0.6	273.1	1926	sch		0	-42.8	-44.3
trichloromethane	CHCl3	pyridine	C5H5N	0.503	336.63	1969	fin	ken	0	9.3	8.8
trichloromethane	CHCl3	cyclopentanone	C5H8O	0.562	308.15	2008	dra	bar	0	-1.1	-2.7
trichloromethane	CHCl3	N-methyl-2-pyrrolidone	C5H9NO	0.494	323.14	1987	wil	wil	0	15.3	13.1
trichloromethane	CHCl3	piperidine	C5H11N	0.867	333.15	2002	fen	vrh	0	3	1.7
trichloromethane	CHCl3	benzene	C6H6	0.82	341.12	1952	buk	maj	0	11.2	11.2
trichloromethane	CHCl3	benzene	C6H6	0.299	342.11	1999	wu	li	0	0.2	0
trichloromethane	CHCl3	4-methyl-2-pentanone	C6H12O	0.94	303.15	2007	cla	mar	0	-2.1	-2.1
trichloromethane	CHCl3	hexane	C6H14	0.601	298.14	1975	bis	wil	0	-3.8	-3.9
trichloromethane	CHCl3	toluene	C7H8	0.865	338.47	1914	ros	bac	0	3.2	3.2
trichloromethane	CHCl3	sulfur dioxide	O2S	0.366	227.61	1975	lor	smi	0	3.6	3.4
dichloromethane	CH2Cl2	methanol	CH4O	0.891	310.33	1963	ten	mis	0	-7.4	-6.2
dichloromethane	CH2Cl2	dimethyl sulfoxide	C2H6OS	0.449	298.14	1973	phi	jam	0	-39.4	-42.6
dichloromethane	CH2Cl2	methyl ethanoate	C3H6O2	0.655	303.14	1973	bye	gib	0	-8.3	-9
dichloromethane	CH2Cl2	tetrahydrofuran	C4H8O	0.078	303.14	1973	bye	gib	0	-1.8	-2.1
dichloromethane	CH2Cl2	1,4-dioxane	C4H8O2	0.645	298.15	1991	nat		0	-4.4	-5
dichloromethane	CH2Cl2	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.275	313.15	1994	kri	vis	1	-3.2	-3.6
methanoic acid	CH2O2	1,2-dichloroethane	C2H4Cl2	0.75	318.13	1960	udo	ale	1	-6.3	-7
methanoic acid	CH2O2	ethanoic acid	C2H4O2	0.161	316.13	1966	kus	tat	1	-1.8	-2
methanoic acid	CH2O2	propanoic acid	C3H6O2	0.263	302.99	1983	tam	dra	0	3.3	2.9
methanoic acid	CH2O2	dimethylformamide	C3H7NO	0.289	369.42	1958	mal	val	0	43.7	44.5

methanoic acid	CH2O2	dipropyl ether	C6H14O	0.938	367.62	1966	hun	sim	0	33.8	34.8
methanoic acid	CH2O2	water	H2O	0.166	313.23	1939	tak		0	21.6	21.1
methanoic acid	CH2O2	water	H2O	0.671	315.43	1958	cha	ale	0	41.2	39.8
methanoic acid	CH2O2	water	H2O	0.316	341.42	1960	riv		0	17	16.3
methanoic acid	CH2O2	water	H2O	0.588	313.03	1966	kus	tat	0	32.4	30.8
silane, trichloromethyl-	CH3Cl3Si	dichloromethylvinylsilane	C3H6Cl2Si	0.581	348.69	2003	yu	qiu	0	0.5	0.5
iodomethane	CH3I	carbon disulfide	CS2	0.249	315.93	1958	gaz	zel	0	6.2	6.5
iodomethane-d3	CH3I	hexane	C6H14	0.182	303.14	1976	wol	goe	2	-8.1	-7.4
formamide	CH3NO	1,4-dioxane	C4H8O2	0.5	323.13	1967	qui		0	-57.3	-47.2
nitromethane	CH3NO2	ethyl ethanoate	C4H8O2	0.552	359.31	1999	tu	ku	0	0.4	1.8
nitromethane	CH3NO2	1-chlorobutane	C4H9Cl	0.506	348.14	1983	khu	mut	2	4.4	2.5
nitromethane	CH3NO2	1-butanol	C4H10O	0.739	313.14	1977	saz	fil	0	-4.6	-1.8
nitromethane	CH3NO2	benzene	C6H6	0.454	298.14	1961	sau	spa	0	3.9	1.6
nitromethane	CH3NO2	ethylbenzene	C8H10	0.257	384.3	1977	bag	kat	1	12.3	9.9
nitromethane	CH3NO2	water	H2O	0.966	296.14	1977	fil	mar	0	-18	-6.8
methanol	CH4O	carbon disulfide	CS2	0.975	326.14	1970	iin	sud	0	-29.1	-30.1
methanol	CH4O	1,1,1-trichloroethane	C2H3Cl3	0.275	328.95	1991	sri	rao	0	-13.9	-13.3
methanol	CH4O	acetonitrile	C2H3N	0.783	326.03	1977	doh	hol	0	-6.7	-1.6
methanol	CH4O	acetonitrile	C2H3N	0.866	336.96	2013	li	bai	0	-4.2	-0.7
methanol	CH4O	1,2-dichloroethane	C2H4Cl2	0.6	313.13	1948	udo	fri	1	-20.2	-19.1
methanol	CH4O	1,1-dichloroethane	C2H4Cl2	0.918	330.38	1988	wis	tam	2	-15	-14.7
methanol	CH4O	N-methylmethanamide	C2H5NO	0.235	313.15	1996	zie		1	-11.2	-83.9
methanol	CH4O	ethanol	C2H6O	0.5	333.12	1921	sch		0	2.6	2.6
methanol	CH4O	ethanol	C2H6O	0.345	345.62	1966	slo	bab	0	-0.6	-0.6
methanol	CH4O	ethanol	C2H6O	0.2	326.39	2006	fuk	mat	0	1.2	1.1
methanol	CH4O	propanenitrile	C3H5N	0.597	341.03	1985	mat	ben	0	-10.1	-4.2
methanol	CH4O	acetone	C3H6O	0.416	328.99	1953	uch	oga	0	-8.7	0.2
methanol	CH4O	acetone	C3H6O	0.4	328.71	1971	och	koj	0	-9	-0.1
methanol	CH4O	acetone	C3H6O	0.22	328.44	1978	och	lu	0	-5.5	1.1
methanol	CH4O	acetone	C3H6O	0.805	332.72	1994	hia	kur	0	-9.6	-1.8
methanol	CH4O	acetone	C3H6O	0.2	328.14	2007	orc	mig	0	-5.2	1.1

methanol	CH4O	propanoic acid	C3H6O2	0.421	318.15	1976	ape	koh	0	1.4	-6.5
methanol	CH4O	methyl ethanoate	C3H6O2	0.36	320.41	1967	dob	bag	0	-16.4	-7.2
methanol	CH4O	methyl ethanoate	C3H6O2	0.943	308.14	1976	fig	web	1	-11.9	-7.2
methanol	CH4O	methyl ethanoate	C3H6O2	0.879	332.73	2011	alv	mat	0	-12.4	-6
methanol	CH4O	dimethyl carbonate	C3H6O3	0.592	321.73	2006	fuk	mat	0	-22.5	-13.8
methanol	CH4O	dimethyl carbonate	C3H6O3	0.788	310.97	2012	yan	zen	0	-16.6	-11.4
methanol	CH4O	dimethylformamide	C3H7NO	0.566	326.58	1963	bit	fle	0	2.7	11.9
methanol	CH4O	2-propanol	C3H8O	0.794	340.79	1991	len	per	0	1.5	1.4
methanol	CH4O	1-propanol	C3H8O	0.3	303.13	1926	sch		0	-4	-4.2
methanol	CH4O	1-propanol	C3H8O	0.352	343.92	2012	mat	fuk	0	3.1	2.9
methanol	CH4O	1,2,3-propanetriol	C3H8O3	0.189	316.35	2013	ven	ben	0	4.3	4.2
methanol	CH4O	thiophene	C4H4S	0.48	313.14	1983	tri		0	-22.4	-21.9
methanol	CH4O	butanenitrile	C4H7N	0.887	339.28	1985	mat	gon	1	-2.2	-1.2
methanol	CH4O	butanone	C4H8O	0.096	308.15	1996	gar	san	1	-9.7	-2.1
methanol	CH4O	ethyloxirane	C4H8O	0.209	298.15	1996	com	fra	2	-15.5	-8.3
methanol	CH4O	butanoic acid	C4H8O2	0.183	308.25	1976	ape	koh	0	-36.7	-59.2
methanol	CH4O	1,4-dioxane	C4H8O2	0.093	308.14	1976	val		0	-33.1	-17.3
methanol	CH4O	ethyl ethanoate	C4H8O2	0.822	323.13	1958	mur	van	0	-11.9	-6.7
methanol	CH4O	ethyl ethanoate	C4H8O2	0.7	335.53	1988	raj	ren	0	-14.5	-7.5
methanol	CH4O	sulfolane	C4H8O2S	0.893	293.15	1969	tom	lin	0	-7	-4.9
methanol	CH4O	diethyl ether	C4H10O	0.05	303.69	1974	sch		0	-9.2	-7.8
methanol	CH4O	2-methyl-1-propanol	C4H10O	0.7	333.12	1948	udo	fri	2	-2.3	-2.5
methanol	CH4O	(RS)-2-butanol	C4H10O	0.932	298.14	1970	pol	mur	0	0.1	0.1
methanol	CH4O	2-ethoxyethanol	C4H10O2	0.94	313.15	2002	deb	bhe	0	0.1	0.2
methanol	CH4O	diethylamine	C4H11N	0.91	339.15	2013	yan	qin	0	12.6	11.5
methanol	CH4O	2-furaldehyde	C5H4O2	0.489	345.77	1987	ni	wan	0	-32.2	-22.7
methanol	CH4O	pyridine	C5H5N	0.903	298.14	1976	nak	ash	0	0.6	1.4
methanol	CH4O	2-methylfuran	C5H6O	0.977	334.32	1950	hic	hal	0	-9.9	-9.6
methanol	CH4O	methyl methacrylate	C5H8O2	0.65	338.98	1974	chu	dan	0	-16.9	-11.6
methanol	CH4O	N-methyl-2-pyrrolidone	C5H9NO	0.846	333.15	1992	bit	eck	0	0.4	2
methanol	CH4O	tetrahydropyran	C5H10O	0.689	321.59	2008	uno	mat	0	-13.3	-7.8

methanol	CH4O	1,1-dimethylethyl methyl ether	C5H12O	0.05	326.29	1979	chu	gor	0	-7.2	-4.6
methanol	CH4O	1,1-dimethylethyl methyl ether	C5H12O	0.159	315	1995	far	lin	0	-13	-7.1
methanol	CH4O	1,1-dimethylethyl methyl ether	C5H12O	0.734	318.15	1996	cot	wie	0	-22.6	-12.8
methanol	CH4O	1,1-dimethylethyl methyl ether	C5H12O	0.635	333.15	1996	tog	tog	0	-21	-11.7
methanol	CH4O	1,1-dimethylethyl methyl ether	C5H12O	0.853	313.15	1999	seg	mar	0	-19.1	-11.1
methanol	CH4O	2-pentanol	C5H12O	0.85	313.15	1996	bar	bhe	0	0.2	0.1
methanol	CH4O	benzene	C6H6	0.7	273.1	1926	sch		0	-25.6	-25.8
methanol	CH4O	benzene	C6H6	0.597	330.58	1954	tal	sch	0	-14.8	-14.4
methanol	CH4O	benzene	C6H6	0.782	331.6	1969	hud	van	0	-14.5	-14.3
methanol	CH4O	benzene	C6H6	0.963	325.76	1973	str	von	0	-8.1	-8
methanol	CH4O	benzene	C6H6	0.701	330.73	1983	rat	sur	0	-16.3	-16
methanol	CH4O	benzene	C6H6	0.687	298.15	1993	miy	hay	0	-18.8	-18.8
methanol	CH4O	2-methylpyridine	C6H7N	0.536	313.14	1977	war		2	10.9	16.5
methanol	CH4O	cyclohexene	C6H10	0.234	328.95	1977	juz	svo	0	-22	-22.4
methanol	CH4O	cyclohexane	C6H12	0.95	328.14	1970	str	svo	0	-18	-18.8
methanol	CH4O	1-methylpropyl ethanoate	C6H12O2	0.883	338.97	2013	wan	xia	0	-2.1	-0.5
methanol	CH4O	hexane	C6H14	0.242	318.13	1932	fer		0	-10.9	-11.8
methanol	CH4O	hexane	C6H14	0.875	323.34	1972	raa	cod	0	-18.1	-19.6
methanol	CH4O	hexane	C6H14	0.759	313.15	1995	ora	war	0	-13.1	-14.3
methanol	CH4O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.163	320	1995	far	lin	0	-22.1	-13.2
methanol	CH4O	dipropyl ether	C6H14O	0.853	323.15	1997	gar	san	0	-10.3	-7.9
methanol	CH4O	ethyl 1,1-dimethylethyl ether	C6H14O	0.844	323.65	2001	wis	aha	0	-14.1	-9.3
methanol	CH4O	toluene	C7H8	0.783	336.83	1972	ish	hir	0	-10	-10.1
methanol	CH4O	2,6-dimethylpyridine	C7H9N	0.799	318.14	1976	nak	ash	0	2.7	3.6
methanol	CH4O	4-heptanone	C7H14O	0.396	298.14	1983	rub	ren	0	-28.9	-16.8
methanol	CH4O	water	H2O	0.398	332.56	1913	wre		0	0.6	-3.8
methanol	CH4O	water	H2O	0.709	331.82	1945	oth	ben	0	-0.9	-2.7
methanol	CH4O	water	H2O	0.7	342.93	1970	les	ogo	4	1.4	-0.4

methanol	CH4O	water	H2O	0.029	308.14	1981	chr	lan	0	7.5	3.8
methanol	CH4O	water	H2O	0.019	298.14	1981	chr	lan	0	7.2	4.1
methanol	CH4O	water	H2O	0.202	318.14	1989	fu	wan	1	1.7	-4.8
methanol	CH4O	water	H2O	0.508	328.15	1995	kur	min	0	0.1	-3.4
methanol	CH4O	water	H2O	0.444	347.47	2011	alv	mat	0	-0.6	-4.3
methanethiol	CH4S	hexane	C6H14	0.383	223.16	1980	wol	szy	0	0.1	0.2
methanamine	CH5N	N,N-dimethylmethanamine	C3H9N	0.798	253.15	1969	wol	wue	0	-9	-6.6
methanamine	CH5N	hexane	C6H14	0.925	228.18	1962	wol	hoe	0	-1	-1.2
carbon monoxide	CO	nitrogen	N2	0.31	79.2	1936	yus	tor	0	1.4	1.1
carbon disulfide	CS2	acetone	C3H6O	0.616	308.3	1900	von		0	-10.3	-10.3
carbon disulfide	CS2	acetone	C3H6O	0.605	313.04	1973	cam	kar	0	-10.9	-10.9
carbon disulfide	CS2	cyclopentane	C5H10	0.075	308.14	1976	ber	bou	0	-3.1	-3.1
carbon disulfide	CS2	benzene	C6H6	0.6	313.13	1926	sch		0	5.8	6
carbon disulfide	CS2	toluene	C7H8	0.7	273.1	1926	sch		0	2.4	2.5
tetrachloroethene	C2Cl4	1,3-dioxacyclopentane	C3H6O2	0.644	315.44	1981	com	cas	0	-6.5	-6.1
tetrachloroethene	C2Cl4	tetrahydrofuran	C4H8O	0.39	313.15	2006	gar	per	0	-3.4	-3.3
tetrachloroethene	C2Cl4	1-butanol	C4H10O	0.961	313.15	1995	dej	bur	0	-7	-6.4
tetrachloroethene	C2Cl4	(RS)-2-butanol	C4H10O	0.114	308.85	1995	dej	bur	0	-15.9	-15.8
tetrachloroethene	C2Cl4	pyridine	C5H5N	0.941	373.12	1967	fri	gal	0	-0.8	-0.6
tetrachloroethene	C2Cl4	1-pentanol	C5H12O	0.11	401.52	1980	rao	rav	0	-12.7	-12.1
tetrachloroethene	C2Cl4	cyclohexane	C6H12	0.838	313.15	2004	gar	pas	0	-9.6	-9.6
trichloroethene	C2HCl3	1,3-dioxacyclopentane	C3H6O2	0.308	337.43	1981	com	cas	0	-8.4	-8.6
trichloroethene	C2HCl3	2-methoxyethanol	C3H8O2	0.022	341.01	1994	jon	sav	0	-7.3	-7.5
trichloroethene	C2HCl3	ethyl ethanoate	C4H8O2	0.302	343.12	1957	rao	rao	1	-1.6	-1.9
trichloroethene	C2HCl3	1-butanol	C4H10O	0.934	314	1996	dej	gon	1	-2.9	-2.3
trichloroethene	C2HCl3	2-methyl-2-propanol	C4H10O	0.385	350.13	1974	han	sub	0	-12.5	-11.8
trichloroethene	C2HCl3	(RS)-2-butanol	C4H10O	0.872	313.26	1996	dej	gon	1	-5.3	-4.4
trichloroethene	C2HCl3	4-methyl-2-pentanone	C6H12O	0.746	365.03	1976	rav	rao	0	-6.1	-6.4
trichloroethene	C2HCl3	butyl ethanoate	C6H12O2	0.803	365.83	1978	rao	rao	2	-1	-1.2
pentafluoroethane	C2HF5	ammonia	H3N	0.951	230.83	2001	yok	zhe	0	2.3	-1.1
(difluoromethoxy)trifluoromethan	C2HF5O	1,1,1-trifluoroethane	C2H3F3	0.6	222.25	2001	kul	des	0	-0.2	0

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(difluoromethoxy)trifluoromethane	C2HF5O	1,1-difluoroethane	C2H4F2	0.4	239.25	2001	kul	des	0	-4.5	-3.6
(difluoromethoxy)trifluoromethane	C2HF5O	fluoroethane	C2H5F	0.6	231.35	2001	kul	des	0	-18	-17.1
(E)-1,2-dichloroethene	C2H2Cl2	acetone	C3H6O	0.157	327.93	1951	alp	elv	1	-8.1	-8.5
(E)-1,2-dichloroethene	C2H2Cl2	cyclopentane	C5H10	0.959	298.14	1985	mac	bou	0	0.5	0.5
1,1,2,2-tetrachloroethane	C2H2Cl4	2-propenol	C3H6O	0.348	342.55	1997	vij	ana	0	-10.9	-10.3
1,1,2,2-tetrachloroethane	C2H2Cl4	2-methoxyethanol	C3H8O2	0.338	401.12	1978	rag	rao	0	-15.9	-16
1,1,2,2-tetrachloroethane	C2H2Cl4	benzene	C6H6	0.467	318.15	2005	gar	per	1	0.5	0.1
1,1,2,2-tetrachloroethane	C2H2Cl4	1-hexene	C6H12	0.517	333.12	1967	han	van	0	-11.4	-11.7
1,1,2,2-tetrachloroethane	C2H2Cl4	hexane	C6H14	0.465	308.14	1987	par	per	0	-2.9	-2.9
1,1,2,2-tetrachloroethane	C2H2Cl4	1-hexanol	C6H14O	0.116	423.95	2010	red	swa	0	-8.6	-7.4
1,1-dichloro-1-fluoroethane	C2H3Cl2F	pentane	C5H12	0.695	300	2013	out	lem	0	-1.6	-1.4
1,1,1-trichloroethane	C2H3Cl3	1,2-dichloroethane	C2H4Cl2	0.662	348.13	1971	sag	san	0	3.1	3.3
1,1,1-trichloroethane	C2H3Cl3	dimethyl carbonate	C3H6O3	0.211	333.15	1994	com	fra	1	-6.3	-6.5
1,1,1-trichloroethane	C2H3Cl3	3-pentanone	C5H10O	0.086	333.15	1998	teo	aim	0	-3.7	-3.7
1,1,1-trichloroethane	C2H3Cl3	benzene	C6H6	0.705	348.83	1977	rao	vis	0	0.3	0.3
1,1,1-trichloroethane	C2H3Cl3	2,2,4-trimethylpentane	C8H18	0.365	343.15	1995	com	fra	5	-3.4	-3.4
2,2,2-trifluoroethanol	C2H3F3O	water	H2O	0.508	298.14	1988	coo	mor	0	6.4	6
acetonitrile	C2H3N	N-methylmethanamide	C2H5NO	0.026	363.15	2003	har	wit	0	-16.1	-25.3
acetonitrile	C2H3N	ethanol	C2H6O	0.217	322.99	1979	wil	pat	0	-16	-8.1
acetonitrile	C2H3N	ethanol	C2H6O	0.608	333.15	2009	com	cre	0	-11.7	-3.3
acetonitrile	C2H3N	1,2-ethanediol	C2H6O2	0.349	323.14	1984	vil	all	2	-71.2	-43.4
acetonitrile	C2H3N	propenenitrile	C3H3N	0.599	351.72	1967	tar	dem	0	-3.4	-3.5
acetonitrile	C2H3N	propanenitrile	C3H5N	0.041	303.29	1987	vil	lan	0	2	2
acetonitrile	C2H3N	propanoic acid	C3H6O2	0.107	298.15	1991	ban	lar	0	-136.7	-125.5
acetonitrile	C2H3N	2-propanol	C3H8O	0.454	349.33	1985	mat	ben	0	-5	2.3
acetonitrile	C2H3N	1-propanol	C3H8O	0.207	343.83	1982	doh	ves	0	-14.3	-4.4
acetonitrile	C2H3N	2-methoxyethanol	C3H8O2	0.474	321.34	1977	cha	nag	1	1.2	5.9
acetonitrile	C2H3N	ethenyl ethanoate	C4H6O2	0.695	347.97	1989	wis	tam	2	-7.7	-7.5

acetonitrile	C2H3N	ethyl ethanoate	C4H8O2	0.148	349	2013	li	cao	0	-3.8	-3.6
acetonitrile	C2H3N	2-methyl-1-propanol	C4H10O	0.826	355.83	1985	mat	gon	1	-2.2	1.5
acetonitrile	C2H3N	chlorobenzene	C6H5Cl	0.161	328.14	1984	nag		0	-29.6	-29.6
acetonitrile	C2H3N	benzene	C6H6	0.367	337.95	1980	aco	rod	0	-12.2	-12.1
acetonitrile	C2H3N	benzene	C6H6	0.66	347.15	1991	dic	maz	0	-8.5	-8.5
acetonitrile	C2H3N	1-hexyne	C6H10	0.493	318.14	1977	des	che	0	-14.6	-14.4
acetonitrile	C2H3N	toluene	C7H8	0.467	357.53	1980	kri	tri	0	-7.7	-7.5
acetonitrile	C2H3N	ethylbenzene	C8H10	0.34	326.95	1991	dic	maz	0	-10.9	-10.6
acetonitrile	C2H3N	2,2,4-trimethylpentane	C8H18	0.061	313.14	1989	van	sve	0	-35.4	-32.4
acetonitrile	C2H3N	water	H2O	0.87	333.12	1950	vie		0	-1.5	6.2
acetonitrile	C2H3N	water	H2O	0.101	322.99	1984	vil	all	1	-63.9	-41.4
ethene	C2H4	cyclohexane	C6H12	0.92	160.01	1979	tif	koh	1	-8.7	-8.7
1,2-dibromoethane	C2H4Br2	1-butanol	C4H10O	0.233	387.75	1995	rod	laf	1	-7.1	-5.6
1,2-dibromoethane	C2H4Br2	benzene	C6H6	0.735	293	1974	bir	vij	0	-5.7	-5.9
1,2-dibromoethane	C2H4Br2	cyclohexane	C6H12	0.887	298.15	1994	kal	sin	0	4.2	5
1,1-dichloroethane	C2H4Cl2	ethanal	C2H4O	0.502	300.14	1989	rou	piv	0	-16.5	-17.1
1,2-dichloroethane	C2H4Cl2	ethanoic acid	C2H4O2	0.704	358.75	2007	has	usl	0	6.7	6.9
1,2-dichloroethane	C2H4Cl2	ethanol	C2H6O	0.512	343.23	1971	sag	san	0	-15.4	-13.1
1,2-dichloroethane	C2H4Cl2	2-propenol	C3H6O	0.42	343.45	1996	vij	ana	1	-13.3	-10.7
1,2-dichloroethane	C2H4Cl2	dimethyl carbonate	C3H6O3	0.4	313.15	1994	com	fra	1	-14.7	-15.3
1,2-dichloroethane	C2H4Cl2	1-propanol	C3H8O	0.7	323.13	1948	udo	fri	2	-4.1	-1.9
1,2-dichloroethane	C2H4Cl2	1-propanol	C3H8O	0.089	361.45	1991	kir	ven	0	-11.9	-10.3
1,2-dichloroethane	C2H4Cl2	2-methyl-1-propanol	C4H10O	0.7	323.13	1948	udo	fri	2	-3.5	-1.2
1,2-dichloroethane	C2H4Cl2	1,1-dimethylethyl methyl ether	C5H12O	0.532	324.74	2008	ami	bou	0	0.1	0.1
1,2-dichloroethane	C2H4Cl2	benzene	C6H6	0.65	355.07	1962	kir	fis	0	3.5	3.4
1,2-dichloroethane	C2H4Cl2	cyclohexane	C6H12	0.271	348.83	1989	mat	gon	0	12.2	12.7
1,2-dichloroethane	C2H4Cl2	hexane	C6H14	0.177	298.14	1988	lop	per	0	7.6	8.2
1,2-dichloroethane	C2H4Cl2	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.863	324.87	2008	ami	bou	0	-5.1	-4.9
1,2-dichloroethane	C2H4Cl2	toluene	C7H8	0.393	349.73	1974	riv		0	7.5	7.5
1,2-dichloroethane	C2H4Cl2	heptane	C7H16	0.365	303.14	1982	gut	kna	0	14	14.7

1,2-dichloroethane	C2H4Cl2	octane	C8H18	0.804	323.15	1990	cha	kat	1	6.4	6.7
ethanal	C2H4O	ethanol	C2H6O	0.3	303.14	1970	dav	sil	0	39.5	47
ethanal	C2H4O	acetone	C3H6O	0.971	294.15	1980	mue	fig	0	0.6	0.6
ethanal	C2H4O	methyl ethanoate	C3H6O2	0.73	299.19	1969	utk	bal	0	-2.5	-2.5
oxirane	C2H4O	water	H2O	0.031	283.14	1955	mac	che	0	-43.1	-15.1
ethanoic acid	C2H4O2	ethanol	C2H6O	0.932	318.14	1980	wag	ape	0	12.3	8.6
ethanoic acid	C2H4O2	acetone	C3H6O	0.239	336.72	1942	yor	hol	0	-1.1	-0.6
ethanoic acid	C2H4O2	acetone	C3H6O	0.12	308.14	1975	war	sur	0	0.7	0.9
ethanoic acid	C2H4O2	propanoic acid	C3H6O2	0.343	404.08	2010	gao	zhu	0	-0.2	-0.2
ethanoic acid	C2H4O2	2-butenal	C4H6O	0.178	348.13	1975	war	sur	0	2	2.6
ethanoic acid	C2H4O2	butanone	C4H8O	0.431	364.66	2009	xie	wan	0	-0.9	0.5
ethanoic acid	C2H4O2	ethyl ethanoate	C4H8O2	0.71	335.12	1955	usa	bil	0	-20.4	-16.8
ethanoic acid	C2H4O2	ethyl ethanoate	C4H8O2	0.021	323.2	2001	miy	nak	1	-4	-4
ethanoic acid	C2H4O2	1-butanol	C4H10O	0.176	391.33	1959	mac		0	13.2	10.5
ethanoic acid	C2H4O2	1-butanol	C4H10O	0.058	358.65	2001	mun	kra	0	8.9	7.3
ethanoic acid	C2H4O2	2-furaldehyde	C5H4O2	0.116	402.04	2003	fel	gri	0	5.9	7.5
ethanoic acid	C2H4O2	propyl ethanoate	C5H10O2	0.591	323.15	2011	fan	li	0	-3.9	-1.6
ethanoic acid	C2H4O2	butyl methyl ether	C5H12O	0.523	355.42	1966	hun	sim	0	2.3	4
ethanoic acid	C2H4O2	benzene	C6H6	0.165	353.52	1967	hau		0	8	8
ethanoic acid	C2H4O2	cyclohexane	C6H12	0.709	318.14	1984	lar	ban	0	36.9	35.6
ethanoic acid	C2H4O2	4-methyl-2-pentanone	C6H12O	0.891	390.96	1993	mal	chy	0	8.7	9.3
ethanoic acid	C2H4O2	butyl ethanoate	C6H12O2	0.94	312.13	1955	usa	bil	0	17.7	18.2
ethanoic acid	C2H4O2	toluene	C7H8	0.615	373.12	1968	mur	rag	0	15.7	15.2
ethanoic acid	C2H4O2	octane	C8H18	0.954	382.93	1958	zie	brz	2	31	29.5
ethanoic acid	C2H4O2	water	H2O	0.197	374.29	1924	pov	mar	0	3.9	4.4
ethanoic acid	C2H4O2	water	H2O	0.072	295.53	1952	oth	sil	0	2.7	2.7
ethanoic acid	C2H4O2	water	H2O	0.187	340.97	1957	cha	ale	1	6.5	6.9
ethanoic acid	C2H4O2	water	H2O	0.124	373.92	1963	ito	yos	0	3.5	3.9
ethanoic acid	C2H4O2	water	H2O	0.491	313.14	1973	laz	mar	0	5.7	6
ethanoic acid	C2H4O2	water	H2O	0.051	343.2	2001	miy	nak	1	3.3	3.5
ethanoic acid	C2H4O2	water	H2O	0.24	374.85	2009	xie	wan	0	4.9	5.5

chloroethane	C2H5Cl	butane	C4H10	0.109	271.8	1957	per		0	0.9	1.1
nitroethane	C2H5NO2	1,3-dichloropropane	C3H6Cl2	0.273	363.15	2011	teo	bar	0	-1.4	-3.1
nitroethane	C2H5NO2	1-methoxy-2-propanol	C4H10O2	0.502	313.15	2006	gil	wil	2	-11.7	-11
nitroethane	C2H5NO2	propyl ethanoate	C5H10O2	0.403	377.56	1999	ku	tu	0	-2.7	-1.7
silane, dichlorodimethyl-	C2H6Cl2Si	silicon tetrachloride	Cl4Si	0.19	330.83	1987	rug	gas	0	0.5	0.7
ethanol	C2H6O	1,2-ethanediol	C2H6O2	0.154	322.99	1983	gon	van	1	-44.1	-44.7
ethanol	C2H6O	propanal	C3H6O	0.603	308.15	1995	cot	pan	0	24.3	31.3
ethanol	C2H6O	acetone	C3H6O	0.938	328.13	1966	vin	sus	0	-10.9	-5.4
ethanol	C2H6O	methyl ethanoate	C3H6O2	0.768	333.13	1970	per	vol	0	-7.9	2.2
ethanol	C2H6O	methyl ethanoate	C3H6O2	0.235	330.49	2011	alv	mat	0	-9.4	-4
ethanol	C2H6O	dimethyl carbonate	C3H6O3	0.845	332.57	2006	fuk	mat	0	-15.1	-9.9
ethanol	C2H6O	2-propanol	C3H8O	0.653	313.14	1989	ora		0	1.4	1.4
ethanol	C2H6O	1-propanol	C3H8O	0.9	343.12	1948	udo	fri	0	-2.6	-2.6
ethanol	C2H6O	1,2,3-propanetriol	C3H8O3	0.75	333.15	2013	ven	ben	0	-11.5	-11.6
ethanol	C2H6O	thiophene	C4H4S	0.058	308.14	1983	tri		0	-24.1	-22.4
ethanol	C2H6O	butanone	C4H8O	0.196	298.15	1996	gar	san	1	-11.1	-4.9
ethanol	C2H6O	1,4-dioxane	C4H8O2	0.551	320.54	1969	man	rad	0	-27.1	-15.1
ethanol	C2H6O	1,4-dioxane	C4H8O2	0.254	308.15	1999	cal	art	0	-34.2	-20.1
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0.051	348.67	1958	mur	van	0	-3.8	-1
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0.459	344.83	1970	kat	kon	0	-16.4	-7.7
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0.203	346.13	1986	ort	pen	0	-11	-4.3
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0.775	345.83	1998	fig	mal	0	-14.5	-7.7
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0.852	323.15	2012	pav	bog	0	-17.1	-10.5
ethanol	C2H6O	methyl propanoate	C4H8O2	0.069	353.4	1990	ort	sus	3	-4.4	-0.7
ethanol	C2H6O	1-bromobutane	C4H9Br	0.398	288.15	2003	gar	mar	0	-19.1	-19
ethanol	C2H6O	1-chlorobutane	C4H9Cl	0.131	288.15	2001	mar	gar	0	-11.5	-10.8
ethanol	C2H6O	1-chlorobutane	C4H9Cl	0.732	333.15	2009	com	cre	0	-15	-14.4
ethanol	C2H6O	diethyl ether	C4H10O	0.699	318.13	1924	lou	bri	0	-15.4	-2.8
ethanol	C2H6O	diethyl ether	C4H10O	0.6	283.14	1935	nag	isi	5	-40.9	-24.3
ethanol	C2H6O	1-butanol	C4H10O	0.968	343.13	1969	kha	per	0	0.3	0.3
ethanol	C2H6O	2-methyl-2-propanol	C4H10O	0.245	355.1	1999	auc	lor	0	3	3

ethanol	C2H6O	2-methyl-1-propanol	C4H10O	0.3	323.13	1948	udo	fri	2	-9	-9.1
ethanol	C2H6O	2-ethoxyethanol	C4H10O2	0.449	313.15	2002	deb	bhe	0	-7	-5.4
ethanol	C2H6O	diethylamine	C4H11N	0.296	334.93	1969	nak	tob	0	0.1	-4.6
ethanol	C2H6O	2-furaldehyde	C5H4O2	0.099	323.14	1970	kha	per	0	-69.3	-32.4
ethanol	C2H6O	pyridine	C5H5N	0.381	348.13	1969	fin	cop	0	-0.7	8.6
ethanol	C2H6O	ethyl propenoate	C5H8O2	0.837	350.53	1968	log	fro	0	-9.3	-6.2
ethanol	C2H6O	N-methyl-2-pyrrolidone	C5H9NO	0.385	333.15	1992	bit	eck	0	6.8	22
ethanol	C2H6O	tetrahydropyran	C5H10O	0.528	331.4	2012	mej	seg	0	-18.5	-10.2
ethanol	C2H6O	1-methylethyl ethanoate	C5H10O2	0.9	351.13	1972	nis		0	-2.2	0.4
ethanol	C2H6O	methyl butanoate	C5H10O2	0.336	356.65	1990	ort	sus	0	-19.1	-9.3
ethanol	C2H6O	1,1-dimethylethyl methyl ether	C5H12O	0.351	329.89	1996	arc	mar	0	-17	-9.3
ethanol	C2H6O	butyl methyl ether	C5H12O	0.104	308.15	2000	hof	spo	0	-7.3	-3.8
ethanol	C2H6O	3-methyl-1-butanol	C5H12O	0.1	343.12	1948	udo	fri	2	-9.2	-9.4
ethanol	C2H6O	chlorobenzene	C6H5Cl	0.59	303.15	1956	sch		0	-17.3	-17.2
ethanol	C2H6O	benzene	C6H6	0.256	335.12	1904	sch		0	-15.9	-14.5
ethanol	C2H6O	benzene	C6H6	0.385	323.13	1952	udo	fat	1	-15.9	-14.7
ethanol	C2H6O	benzene	C6H6	0.266	328.13	1963	yua	lu	0	-14.5	-13.3
ethanol	C2H6O	benzene	C6H6	0.53	298.14	1977	hwa	rob	0	-16.9	-16
ethanol	C2H6O	benzene	C6H6	0.745	303.15	1990	zie	ora	0	-22.9	-22.2
ethanol	C2H6O	2-methylpyridine	C6H7N	0.13	313.14	1977	war		2	-4.7	10
ethanol	C2H6O	cyclohexane	C6H12	0.85	303.13	1935	nag	isi	1	-15.9	-17
ethanol	C2H6O	cyclohexane	C6H12	0.951	345.6	1963	yua	lu	0	-9.5	-9.8
ethanol	C2H6O	cyclohexane	C6H12	0.069	298.15	1995	cot	pan	0	-10.9	-11.2
ethanol	C2H6O	propyl propanoate	C6H12O2	0.886	352.37	1994	ort	gal	0	-4.6	-3.4
ethanol	C2H6O	butyl ethanoate	C6H12O2	0.531	358.78	1987	ort	pen	0	-13.8	-7
ethanol	C2H6O	hexane	C6H14	0.591	328.35	1963	ho	lu	0	-12.5	-12.8
ethanol	C2H6O	hexane	C6H14	0.096	323.14	1976	wol	goe	0	-8.8	-8.7
ethanol	C2H6O	hexane	C6H14	0.938	318.14	1986	osh	sto	0	-19.8	-20.8
ethanol	C2H6O	dipropyl ether	C6H14O	0.354	288.15	1997	gar	per	0	-24.2	-16.3
ethanol	C2H6O	ethyl 1,1-dimethylethyl ether	C6H14O	0.694	338.15	1999	rar	hor	0	-24.2	-16

ethanol	C2H6O	triethylamine	C6H15N	0.844	307.98	1953	cop	eve	0	2.7	6.1
ethanol	C2H6O	toluene	C7H8	0.904	343.12	1933	wri		0	-9.3	-9.2
ethanol	C2H6O	toluene	C7H8	0.623	313.14	1980	ora	kol	0	-15	-14.7
ethanol	C2H6O	toluene	C7H8	0.251	336.56	2007	uno	kik	0	-23.1	-21.9
ethanol	C2H6O	heptane	C7H16	0.4	343.13	1968	ram	del	0	-13.2	-13.6
ethanol	C2H6O	heptane	C7H16	0.66	344.33	1972	raa	cod	0	-10.2	-10.5
ethanol	C2H6O	heptane	C7H16	0.429	303.26	1982	ber	rog	0	-10.7	-11.4
ethanol	C2H6O	1,4-dimethylbenzene	C8H10	0.9	346.03	2011	mat	yam	0	-3.7	-3.6
ethanol	C2H6O	2,4,4-trimethyl-1-pentene	C8H16	0.297	343.48	2003	pok	reh	0	-16.4	-16.2
ethanol	C2H6O	octane	C8H18	0.521	343.15	1995	hia	tak	1	-12.4	-13
ethanol	C2H6O	2,2,4-trimethylpentane	C8H18	0.377	298.14	1948	kre	now	0	-11.1	-11.8
ethanol	C2H6O	water	H2O	0.262	312.89	1910	vre		0	-3.6	-9.6
ethanol	C2H6O	water	H2O	0.167	298.14	1925	dob		0	-3.7	-11.1
ethanol	C2H6O	water	H2O	0.013	322.23	1939	kir	ger	1	5.4	2.5
ethanol	C2H6O	water	H2O	0.25	338.12	1948	rao	ach	0	-4.7	-10.2
ethanol	C2H6O	water	H2O	0.149	357.62	1953	ots	wil	0	-0.7	-6
ethanol	C2H6O	water	H2O	0.207	303.13	1960	gar	sta	0	-4.9	-11.8
ethanol	C2H6O	water	H2O	0.921	319.98	1969	koj	kat	0	-1.1	-2
ethanol	C2H6O	water	H2O	0.685	328.14	1972	mer		0	-3.4	-6.4
ethanol	C2H6O	water	H2O	0.16	357.05	1972	sta	met	0	-2.4	-7.7
ethanol	C2H6O	water	H2O	0.493	353.03	1976	pau		0	-3.1	-6.7
ethanol	C2H6O	water	H2O	0.15	333.13	1980	bel	voh	0	-1	-7.1
ethanol	C2H6O	water	H2O	0.023	308.14	1984	nor	tuc	0	9	4.6
ethanol	C2H6O	water	H2O	0.05	308.14	1984	nor	tuc	0	8.4	2.5
ethanol	C2H6O	water	H2O	0.075	308.14	1984	nor	tuc	0	5.3	-1.3
ethanol	C2H6O	water	H2O	0.099	308.14	1984	nor	tuc	0	2.1	-4.9
ethanol	C2H6O	water	H2O	0.02	298.14	1984	nor	tuc	0	10.3	6.1
ethanol	C2H6O	water	H2O	0.064	298.14	1984	nor	tuc	0	9.1	2.5
ethanol	C2H6O	water	H2O	0.107	298.14	1984	nor	tuc	0	2.5	-4.8
ethanol	C2H6O	water	H2O	0.229	298.14	1984	nor	tuc	0	-5.8	-12.7
ethanol	C2H6O	water	H2O	0.176	323.15	1995	kur	min	0	-3.9	-10.3

ethanol	C2H6O	water	H2O	0.115	358.79	2002	wan	yan	0	0.1	-5.3
ethanol	C2H6O	water	H2O	0.945	315.13	2011	vou	pam	0	-0.1	-0.7
dimethyl ether	C2H6O	sulfur dioxide	O2S	0.928	243.07	1966	pup	rib	0	4.3	4.2
dimethyl sulfoxide	C2H6OS	acetone	C3H6O	0.801	308.14	1974	sas	kon	0	-36.1	-36.8
dimethyl sulfoxide	C2H6OS	tetrahydrofuran	C4H8O	0.1	318.14	1974	sas	kon	0	-0.8	-0.8
dimethyl sulfoxide	C2H6OS	1,4-dioxane	C4H8O2	0.422	333.15	1992	iul	lan	1	-19.5	-19.5
dimethyl sulfoxide	C2H6OS	1,4-dioxane	C4H8O2	0.8	333.15	1997	iul	ham	0	-29.4	-29.8
dimethyl sulfoxide	C2H6OS	2-methyl-1-propanol	C4H10O	0.584	365.63	1972	bet	mcm	0	-22.1	-0.4
dimethyl sulfoxide	C2H6OS	benzene	C6H6	0.953	313.13	1960	ken	lin	1	-137.8	-141.7
dimethyl sulfoxide	C2H6OS	water	H2O	0.035	333.28	1989	lan	iul	0	0.2	0.1
dimethyl sulfoxide	C2H6OS	water	H2O	0.734	296.09	1995	lai	lau	0	-33.1	18.9
1,2-ethanediol	C2H6O2	1,2-propanediol	C3H8O2	0.524	359.93	1972	sok	tsy	1	-6	-6
1,2-ethanediol	C2H6O2	bis(2-hydroxyethyl)amine	C4H11NO2	0.103	433.11	1987	wil	wil	2	8.5	7.7
1,2-ethanediol	C2H6O2	N-methylbenzenamine	C7H9N	0.96	393.13	1957	cru	jos	0	-36.7	-36.9
1,2-ethanediol	C2H6O2	water	H2O	0.054	359.12	1935	tri	pot	0	-0.3	-0.4
1,2-ethanediol	C2H6O2	water	H2O	0.316	363.43	1983	nat	ben	0	7	4.9
1,2-ethanediol	C2H6O2	water	H2O	0.242	353.15	2004	hor	gar	0	4.1	2.6
2,3-dithiabutane	C2H6S2	2,4,4-trimethyl-1-pentene	C8H16	0.086	368.15	2010	sap	uus	2	-2.4	-2.3
ethylamine	C2H7N	butane	C4H10	0.168	233.18	1964	wol	hoe	0	1.4	-1.3
N-methylmethanamine	C2H7N	hexane	C6H14	0.512	253.17	1966	wol	hoe	0	-12.4	-14.2
2-aminoethanol	C2H7NO	water	H2O	0.015	363.15	1990	len	rou	0	0.9	0.9
2-aminoethanol	C2H7NO	water	H2O	0.202	303.15	2009	bel	raz	0	12.9	11.2
1,2-ethanediamine	C2H8N2	toluene	C7H8	0.968	381.12	1985	cha	kat	1	-13.8	-18.3
1,2-ethanediamine	C2H8N2	1,2-dimethylbenzene	C8H10	0.439	370.02	1977	car	mar	0	7.6	-4.8
1,2-ethanediamine	C2H8N2	water	H2O	0.168	364.27	1973	sch	qui	0	24.9	20.6
propenenitrile	C3H3N	2-propenal	C3H4O	0.624	319.03	1965	sok	sev	0	-4.9	-4.8
propenenitrile	C3H3N	1-propanol	C3H8O	0.629	351.83	1985	mat	gon	0	-7.1	-0.8
propenenitrile	C3H3N	hexane	C6H14	0.961	308.6	1996	deh	boe	0	2.1	2.7
1-chloro-2,3-epoxypropane	C3H5ClO	ethylbenzene	C8H10	0.359	398.05	2005	vit	val	0	14.2	14.3
1-chloro-2,3-epoxypropane	C3H5ClO	water	H2O	0.521	361.7	2009	yue	zhu	0	-2.8	4.7

propanenitrile	C3H5N	2-propanol	C3H8O	0.808	360.68	1985	mat	gon	1	-9.9	-2.4
propanenitrile	C3H5N	benzene	C6H6	0.825	318.15	1995	art	mun	2	-10.9	-11
propanenitrile	C3H5N	ethyl 1,1-dimethylethyl ether	C6H14O	0.988	312.86	2010	hai	uus	1	-4.8	-4.7
1,3-dichloropropane	C3H6Cl2	acetone	C3H6O	0.723	313.15	1998	dra	bar	0	-10.4	-10.9
1,2-dichloropropane	C3H6Cl2	propanal	C3H6O	0.732	308.14	1977	bou	jad	0	-11.3	-11.7
acetone	C3H6O	methyl ethanoate	C3H6O2	0.504	328.78	1980	muh	fig	0	-2.7	-2.7
acetone	C3H6O	methyl ethanoate	C3H6O2	0.606	323.14	1981	ols		0	-2.8	-2.8
acetone	C3H6O	2-propanol	C3H8O	0.571	334.99	1989	gul		0	-11.5	-3.8
2-propenol	C3H6O	1-propanol	C3H8O	0.078	333.15	2004	lub	mal	0	0.8	0.8
acetone	C3H6O	2-methoxyethanol	C3H8O2	0.835	321.34	1979	cha	nag	0	-5.7	-4.5
acetone	C3H6O	butanone	C4H8O	0.276	303.15	1995	cam	bhe	0	-1.4	-1.4
propanal	C3H6O	butanone	C4H8O	0.017	318.14	1973	mat	kat	0	-1.7	-1.7
methyloxirane	C3H6O	2-methyl-2-propanol	C4H10O	0.65	315.24	1974	vos	kom	0	-7.1	-1.8
acetone	C3H6O	benzene	C6H6	0.837	330.63	1901	ebe		0	-2.5	-2.6
acetone	C3H6O	benzene	C6H6	0.533	303.14	1971	kra	lin	0	-12.5	-12.7
acetone	C3H6O	phenol	C6H6O	0.1	323.13	1963	goe		0	-145	-100.7
acetone	C3H6O	cyclohexane	C6H12	0.39	328.13	1957	rao	rao	2	-12.7	-12.5
acetone	C3H6O	cyclohexane	C6H12	0.482	313.15	1992	gor	ora	0	-13.1	-13
2-propenol	C3H6O	cyclohexane	C6H12	0.121	333.15	2002	lub	ban	0	-1.4	-1.2
acetone	C3H6O	hexane	C6H14	0.431	322.85	1961	ogo	kog	5	-15.7	-15.4
acetone	C3H6O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.612	327.75	1995	res	bet	0	-13	-12.9
acetone	C3H6O	triethylamine	C6H15N	0.042	318.14	1985	kie	bit	0	-20.8	-20.5
acetone	C3H6O	toluene	C7H8	0.131	318.13	1965	ory	pra	0	-29	-29.2
acetone	C3H6O	4-methylphenol	C7H8O	0.8	339.62	1936	pia		0	4.6	5.7
acetone	C3H6O	2,2,4-trimethylpentane	C8H18	0.31	303.13	1964	edw	sch	0	-16.7	-16.3
acetone	C3H6O	water	H2O	0.171	319.13	1902	sch		0	-43.5	-15
acetone	C3H6O	water	H2O	0.427	334.22	1949	gri	buf	0	-13.7	2.9
acetone	C3H6O	water	H2O	0.3	303.14	1973	dav	cot	0	-36	-9.3
acetone	C3H6O	water	H2O	0.1	318.14	1982	wan	tan	1	-47.1	-19.3
acetone	C3H6O	water	H2O	0.603	332.55	2000	gu	hou	0	-6.9	4.5

2-propenol	C3H6O	water	H2O	0.574	361.72	1957	har	moo	0	-1.9	-4
methyl ethanoate	C3H6O2	2-propanol	C3H8O	0.712	332.57	1993	ort	sus	0	-7.8	-2.4
methyl ethanoate	C3H6O2	1-propanol	C3H8O	0.9	318.14	1976	nag	oht	1	-0.4	1.1
methyl ethanoate	C3H6O2	tetrahydrofuran	C4H8O	0.904	330.37	1996	wis		9	0.7	0.6
methyl ethanoate	C3H6O2	ethyloxirane	C4H8O	0.014	336.2	1997	mon	wis	0	-0.5	-0.5
propanoic acid	C3H6O2	butanoic acid	C4H8O2	0.576	413.15	2006	gil	wil	2	3	3
propanoic acid	C3H6O2	2-methylpropanoic acid	C4H8O2	0.6	417.62	1972	tat	kus	0	-3.6	-3.6
methyl ethanoate	C3H6O2	ethyl ethanoate	C4H8O2	0.6	333.12	1921	sch		0	-6.2	-6.2
1,3-dioxacyclopentane	C3H6O2	1,4-dioxane	C4H8O2	0.206	337.73	1984	cas	fra	0	-7.6	-7.6
1,3-dioxacyclopentane	C3H6O2	2-chlorobutane	C4H9Cl	0.667	342.33	1994	wis	ape	3	-5.6	-5.6
1,3-dioxacyclopentane	C3H6O2	2-methyl-2-propanol	C4H10O	0.888	322.95	2004	rey	laf	0	-4.5	-1.4
1,3-dioxacyclopentane	C3H6O2	2-methyl-1-propanol	C4H10O	0.624	354.83	2004	rey	laf	0	-11.7	-4.7
methyl ethanoate	C3H6O2	2-methyl-1-propanol	C4H10O	0.508	332.58	1995	sus		0	-13.6	-4.5
propanoic acid	C3H6O2	ethyl propanoate	C5H10O2	0.674	358.17	1982	mac	ras	0	-8.5	-5.7
methyl ethanoate	C3H6O2	1,1-dimethylethyl methyl ether	C5H12O	0.701	324.55	1997	wis	emb	1	-0.5	-0.6
1,3-dioxacyclopentane	C3H6O2	chlorobenzene	C6H5Cl	0.506	356.53	1985	fra	com	3	-17.7	-18.1
methyl ethanoate	C3H6O2	benzene	C6H6	0.5	313.13	1921	sch		0	-13.9	-14.2
methyl ethanoate	C3H6O2	benzene	C6H6	0.761	313.14	1973	nag	oht	1	-7	-7.1
propanoic acid	C3H6O2	cyclohexane	C6H12	0.609	361.53	1980	svi	mal	0	25.4	24.7
1,3-dioxacyclopentane	C3H6O2	cyclohexane	C6H12	0.879	313.14	1989	wu	san	0	-6.8	-6.8
ethyl methanoate	C3H6O2	hexane	C6H14	0.359	325.6	2007	ort	sab	0	4.9	5
1,3-dioxacyclopentane	C3H6O2	hexane	C6H14	0.4	308.15	1999	cal	art	0	-3.5	-3.2
methyl ethanoate	C3H6O2	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.744	326.15	1996	wis	bla	0	-3.9	-4
1,3-dioxacyclopentane	C3H6O2	methylcyclohexane	C7H14	0.045	313.14	1988	cas	fra	0	5	5.5
propanoic acid	C3H6O2	heptane	C7H16	0.892	323.14	1981	sch		1	51.2	49.6
1,3-dioxacyclopentane	C3H6O2	1,3-dimethylbenzene	C8H10	0.31	341.33	1982	cas	fra	0	-16.7	-16.8
propanoic acid	C3H6O2	water	H2O	0.956	370.02	1961	riv		0	2.5	1.6
propanoic acid	C3H6O2	water	H2O	0.74	353.13	1978	raf	har	0	-20.6	-20.8
1,3-dioxacyclopentane	C3H6O2	water	H2O	0.55	323.14	1979	hrn	mat	0	-26.8	-10.2
dimethyl carbonate	C3H6O3	2-propanol	C3H8O	0.401	345.71	2012	mat	fuk	0	-14	-6.4

dimethyl carbonate	C3H6O3	1-propanol	C3H8O	0.85	334.74	2012	mat	fuk	0	-9.4	-4.6
dimethyl carbonate	C3H6O3	(RS)-2-butanol	C4H10O	0.749	343.49	2012	mat	fuk	0	-7.1	-1.5
dimethyl carbonate	C3H6O3	2-pentanone	C5H10O	0.121	372.33	2005	per	rod	1	-0.5	-0.6
dimethyl carbonate	C3H6O3	cyclohexane	C6H12	0.803	333.15	1993	neg	blo	0	3.8	3.6
dimethyl carbonate	C3H6O3	toluene	C7H8	0.053	318.13	1965	ory	pra	0	-1.2	-1.3
dimethyl carbonate	C3H6O3	heptane	C7H16	0.439	355.95	2002	rod	can	1	7.4	7.4
1-chloropropane	C3H7Cl	butanone	C4H8O	0.655	327.94	1971	gar	mir	0	2.1	2.1
1-chloropropane	C3H7Cl	tetrahydrofuran	C4H8O	0.493	329.01	2009	gin	mon	0	0	-0.1
1-chloropropane	C3H7Cl	tetrahydropyran	C5H10O	0.937	310.52	2009	gin	mon	0	0.6	0.6
dimethylformamide	C3H7NO	1-butanol	C4H10O	0.379	338.15	1991	wil	wil	0	-4.1	4.3
dimethylformamide	C3H7NO	2-methyl-1-propanol	C4H10O	0.382	389.35	2006	pra	sra	0	-7.8	-1.1
N-methylacetamide	C3H7NO	pyridine	C5H5N	0.704	398.6	1997	deh	fis	1	-14.7	-15.3
dimethylformamide	C3H7NO	2-methyl-1-butanol	C5H12O	0.454	409.58	2013	zhu	yao	0	-13.4	-5.3
dimethylformamide	C3H7NO	1-pentanol	C5H12O	0.549	397.05	1995	mar	gab	0	-5.6	3
dimethylformamide	C3H7NO	bromobenzene	C6H5Br	0.377	421.05	2008	pra	red	0	-15.6	-15.9
dimethylformamide	C3H7NO	2-methylpropyl ethanoate	C6H12O2	0.226	392.76	2005	mun	mon	0	-7.4	-7.4
dimethylformamide	C3H7NO	1-chlorohexane	C6H13Cl	0.537	313.15	2007	gar	emb	0	-21.3	-21.5
dimethylformamide	C3H7NO	triethylamine	C6H15N	0.341	323.14	1985	kie	bit	0	-17.7	-17.5
dimethylformamide	C3H7NO	toluene	C7H8	0.317	353.2	2000	zhe	zho	0	-11.3	-11.3
dimethylformamide	C3H7NO	1,4-dimethylbenzene	C8H10	0.1	409.35	1987	bag	rat	0	-7.3	-7.3
dimethylformamide	C3H7NO	water	H2O	0.371	365.02	1961	sus		0	8.7	13.9
dimethylformamide	C3H7NO	water	H2O	0.5	333.13	1978	mis	smi	0	-6.8	5.1
dimethylformamide	C3H7NO	water	H2O	0.926	343.15	1995	iul	ham	0	-6.1	18.8
N-methylacetamide	C3H7NO	water	H2O	0.22	353.13	1975	man	kor	0	6	3.5
2-nitropropane	C3H7NO2	cyclohexane	C6H12	0.055	318.14	1979	mar	fre	0	-2.8	-2.9
1-nitropropane	C3H7NO2	heptane	C7H16	0.643	372.42	1973	tol	kog	0	-6.5	-7.2
propane	C3H8	hydrogen sulfide	H2S	0.297	182.33	2006	lob	fer	0	6.6	6.4
2-propanol	C3H8O	1-propanol	C3H8O	0.973	313.14	1989	ora		0	0.2	0.2
2-propanol	C3H8O	2-methoxyethanol	C3H8O2	0.767	359.48	2007	lla	mon	2	-4.5	-4.1
1-propanol	C3H8O	2-methoxyethanol	C3H8O2	0.458	378.92	1977	cha	nag	0	-9.9	-8.7
1-propanol	C3H8O	thiophene	C4H4S	0.926	313.14	1983	tri		0	-26.7	-25.7

2-propanol	C3H8O	butanone	C4H8O	0.652	313.15	1996	gar	san	3	-19.3	-9.6
1-propanol	C3H8O	butanone	C4H8O	0.249	323.15	1996	gar	san	3	-7.3	-2.3
2-propanol	C3H8O	1,4-dioxane	C4H8O2	0.442	353.15	1998	rao	rav	0	-22.8	-12
2-propanol	C3H8O	ethyl ethanoate	C4H8O2	0.599	349.97	1958	mur	van	0	-8.2	-0.8
2-propanol	C3H8O	methyl propanoate	C4H8O2	0.763	350.93	1993	ort	sus	0	-10.7	-4.4
1-propanol	C3H8O	propyl methanoate	C4H8O2	0.9	364.72	1967	moz	mit	1	-9.8	-5.1
1-propanol	C3H8O	methyl propanoate	C4H8O2	0.08	355.79	1990	ort	sus	3	-2.1	0
1-propanol	C3H8O	2-methyl-1-propanol	C4H10O	0.114	323.13	1948	udo	fri	1	-1.5	-1.6
1-propanol	C3H8O	1-butanamine	C4H11N	0.767	313.14	1976	cho		0	24.6	12.8
1-propanol	C3H8O	N-methyl-2-pyrrolidone	C5H9NO	0.944	333.15	1994	bit	eck	0	0.4	0.6
2-propanol	C3H8O	3-pentanone	C5H10O	0.786	357.33	1989	ste	kuk	0	-1.5	1.7
1-propanol	C3H8O	tetrahydropyran	C5H10O	0.151	353.33	2008	uno	mat	0	-6.8	-3.1
2-propanol	C3H8O	ethyl propanoate	C5H10O2	0.8	343	2012	sun	gor	0	-10.7	-6.8
2-propanol	C3H8O	1-methylethyl ethanoate	C5H10O2	0.8	354.03	1971	nis		0	-6.7	-2.3
2-propanol	C3H8O	propyl ethanoate	C5H10O2	0.833	351.55	1999	gon	ort	0	-24.3	-20.8
2-propanol	C3H8O	butyl methanoate	C5H10O2	0.441	359.5	1996	gon	ort	6	-13	-6.2
1-propanol	C3H8O	propyl ethanoate	C5H10O2	0.905	369.32	1959	pic	hal	0	-3.3	-0.7
1-propanol	C3H8O	propyl ethanoate	C5H10O2	0.04	373.47	2000	ort	gon	0	-1.3	0.9
1-propanol	C3H8O	methyl butanoate	C5H10O2	0.589	333.13	1985	fer	ber	0	-18.4	-9.8
1-propanol	C3H8O	2-methyl-1-butanol	C5H12O	0.935	371.43	2006	res	gon	0	0.1	0
1-propanol	C3H8O	1-pentanol	C5H12O	0.688	361.01	1983	vil		0	-0.6	-0.6
1-propanol	C3H8O	chlorobenzene	C6H5Cl	0.838	347.12	1960	ell	mcd	0	-6	-5.6
2-propanol	C3H8O	benzene	C6H6	0.36	333.32	1965	nag		0	-11.4	-9.9
2-propanol	C3H8O	benzene	C6H6	0.932	351.56	1973	toj	bao	0	-8.3	-7.8
2-propanol	C3H8O	benzene	C6H6	0.35	313.15	2001	rho	gri	0	-14.8	-13.5
1-propanol	C3H8O	benzene	C6H6	0.359	321.73	1947	bri	nut	0	-12.7	-11.2
1-propanol	C3H8O	benzene	C6H6	0.124	350.38	1973	toj	bao	0	-3.8	-2.4
1-propanol	C3H8O	benzene	C6H6	0.494	340.12	1975	str	svo	0	-12.4	-10.6
1-propanol	C3H8O	benzene	C6H6	0.937	313.14	1987	ora	kol	0	-20	-19.1
1-propanol	C3H8O	benzene	C6H6	0.589	342.45	2008	mej	seg	0	-18.3	-16.4
2-propanol	C3H8O	cyclohexane	C6H12	0.484	342.32	1963	yua	lu	0	-7.5	-7.5

2-propanol	C3H8O	cyclohexane	C6H12	0.732	298.15	1996	gup	mak	0	-17.7	-18.5
1-propanol	C3H8O	cyclohexane	C6H12	0.762	338.13	1970	str	svo	0	-12.8	-13
1-propanol	C3H8O	cyclohexane	C6H12	0.152	333.15	1997	kur	uch	0	-5.9	-5.6
1-propanol	C3H8O	propyl propanoate	C6H12O2	0.53	372.12	1967	moz	mit	1	-20.3	-13
1-propanol	C3H8O	butyl ethanoate	C6H12O2	0.518	375.78	1995	gon	ort	1	-10.9	-4
2-propanol	C3H8O	hexane	C6H14	0.278	335.03	1976	gov	and	0	-5.8	-5.5
2-propanol	C3H8O	hexane	C6H14	0.983	323.14	1988	mac	fra	0	-6.6	-6.8
1-propanol	C3H8O	hexane	C6H14	0.705	298.14	1982	sch	ale	0	-20.6	-21.3
2-propanol	C3H8O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.342	339.45	1940	mil	bli	0	-21.9	-14.4
2-propanol	C3H8O	dipropyl ether	C6H14O	0.357	293.15	1997	gar	san	2	-21.2	-14.2
2-propanol	C3H8O	ethyl 1,1-dimethylethyl ether	C6H14O	0.21	333.75	2002	seg	mej	0	-17.6	-11.8
1-propanol	C3H8O	dipropyl ether	C6H14O	0.084	278.15	1997	gar	san	2	-6.3	-4.1
1-propanol	C3H8O	ethyl 1,1-dimethylethyl ether	C6H14O	0.268	326.84	2007	mej	seg	0	-15	-9.1
2-propanol	C3H8O	4-methyl-3,5-dioxaheptane	C6H14O2	0.458	353.32	2005	kim	sap	0	-19.1	-10.1
2-propanol	C3H8O	triethylamine	C6H15N	0.712	303.19	1974	chu	dru	0	-1.9	3.7
1-propanol	C3H8O	triethylamine	C6H15N	0.338	283.15	1974	chu	dru	0	-5.8	2.6
2-propanol	C3H8O	toluene	C7H8	0.38	362.35	2012	che	zho	0	-11.9	-10.6
2-propanol	C3H8O	heptane	C7H16	0.112	303.13	1967	van	soc	0	-10.3	-10.4
2-propanol	C3H8O	heptane	C7H16	0.498	313.15	2002	cha	seg	0	-8.2	-8.5
1-propanol	C3H8O	heptane	C7H16	0.499	303.13	1967	van	soc	0	-11.6	-11.7
1-propanol	C3H8O	heptane	C7H16	0.907	288.15	1980	sip	wie	0	-26.3	-27.5
1-propanol	C3H8O	heptane	C7H16	0.84	313.15	1992	zie		0	-17.5	-18.1
1-propanol	C3H8O	benzene, ethenyl-	C8H8	0.942	311.93	1957	mal	mal	0	-4.4	-4.2
1-propanol	C3H8O	ethylbenzene	C8H10	0.664	371.42	1954	ell	fro	0	-7.7	-7.1
2-propanol	C3H8O	2,2,4-trimethylpentane	C8H18	0.171	340	2008	psu	wic	0	-8.2	-7.9
1-propanol	C3H8O	octane	C8H18	0.582	313.14	1976	ora		0	-11.2	-11.5
1-propanol	C3H8O	2,2,4-trimethylpentane	C8H18	0.501	328.36	1981	ber	nea	0	-10	-9.8
2-propanol	C3H8O	water	H2O	0.025	362.12	1948	dun		0	5.3	-0.7
2-propanol	C3H8O	water	H2O	0.031	333.12	1967	udo	maz	0	8.9	1.8
2-propanol	C3H8O	water	H2O	0.714	353.26	1970	ver		2	-2.9	-6

2-propanol	C3H8O	water	H2O	0.175	348.22	1975	sad	mor	0	-0.2	-6.2
2-propanol	C3H8O	water	H2O	0.032	298.14	1984	nor	tuc	0	18.5	11.1
2-propanol	C3H8O	water	H2O	0.069	298.14	1984	nor	tuc	0	8.1	-0.5
2-propanol	C3H8O	water	H2O	0.024	308.14	1984	nor	tuc	0	16.4	9.5
2-propanol	C3H8O	water	H2O	0.052	308.14	1984	nor	tuc	0	10.4	2.1
2-propanol	C3H8O	water	H2O	0.079	308.14	1984	nor	tuc	0	4.5	-4.1
2-propanol	C3H8O	water	H2O	0.7	349.63	1986	zha	wan	0	-0.6	-3.7
2-propanol	C3H8O	water	H2O	0.689	353.28	2003	arc	arc	0	-2.8	-6
1-propanol	C3H8O	water	H2O	0.432	360.92	1910	dor	pol	0	-1.6	-5.1
1-propanol	C3H8O	water	H2O	0.482	360.92	1958	mur	van	0	-1.8	-5.4
1-propanol	C3H8O	water	H2O	0.7	361.92	1968	koj	toc	0	-3.3	-7
1-propanol	C3H8O	water	H2O	0.496	350.73	1979	goe	sti	0	-1.5	-5.3
1-propanol	C3H8O	water	H2O	0.177	332.08	1996	gab	mar	0	-5.4	-10.1
1,3-propanediol	C3H8O2	1,2,3-propanetriol	C3H8O3	0.15	441.99	2012	mok	saw	0	-15.9	-16.1
1,2-propanediol	C3H8O2	1,2-propanediyl carbonate	C4H6O3	0.622	403.87	2011	mat	kim	0	-15.3	-8.9
1,2-propanediol	C3H8O2	1,2-butanediol	C4H10O2	0.122	403.29	2013	zha	wu	0	-3.8	-3.8
2-methoxyethanol	C3H8O2	2-(N,N-dimethylamino)ethanol	C4H11NO	0.554	346.74	1970	qui	hof	0	5.1	4.2
2-methoxyethanol	C3H8O2	cyclohexane	C6H12	0.019	352.34	2010	mar	lor	0	-1	-0.8
2-methoxyethanol	C3H8O2	heptane	C7H16	0.701	323.15	2001	car	bhe	0	-25.3	-26.3
2-methoxyethanol	C3H8O2	ethylbenzene	C8H10	0.522	392.22	1977	kum	raj	0	-11	-10.8
1,2-propanediol	C3H8O2	water	H2O	0.026	318.14	1975	ver	ver	0	0.5	0.4
1,2,3-propanetriol	C3H8O3	water	H2O	0.601	333.13	1970	var	ste	0	15.8	10.7
1,2,3-propanetriol	C3H8O3	water	H2O	0.133	329.31	2011	coe	dos	0	7.2	6.4
1-propanethiol	C3H8S	benzene	C6H6	0.279	333.13	1989	mcn	wil	0	22.5	22.6
1-propanethiol	C3H8S	hexane	C6H14	0.065	340.76	1949	den	fid	0	0.4	0.5
2-propanamine	C3H9N	hexane	C6H14	0.515	303.14	1983	wol	sha	0	5.3	2.5
1-propanamine	C3H9N	hexane	C6H14	0.429	323.14	1983	wol	sha	0	7.2	3.2
2-(methylamino)ethanol	C3H9NO	N-methyldiethanolamine	C5H13NO2	0.75	351.13	1989	smi	ter	0	1	0.4
trimethyl phosphite	C3H9O3P	benzene	C6H6	0.4	324.35	1990	dut	kah	0	0.3	0.3
1,3-propanediamine	C3H10N2	water	H2O	0.744	303.15	2011	ahm	neg	0	8.7	-46

1-buten-3-yne	C4H4	ammonia	H3N	0.14	218.19	1964	sha	bra	0	-12.1	-14.9
thiophene	C4H4S	pyridine	C5H5N	0.385	370.57	1979	sus		0	-10	-10
thiophene	C4H4S	benzene	C6H6	0.496	328.14	1971	kud	vii	0	-3.8	-3.8
thiophene	C4H4S	2,3-dimethyl-2-butene	C6H12	0.408	347.34	2012	bai	guo	0	-4.4	-4.1
thiophene	C4H4S	toluene	C7H8	0.604	361.32	2006	erl	zay	0	-0.8	-0.8
thiophene	C4H4S	methylcyclohexane	C7H14	0.426	348.13	1980	dia	cre	0	2.7	3.1
pyrrole	C4H5N	1-butanol	C4H10O	0.312	366.6	2012	zaw	nge	0	-30.1	-29.2
pyrrole	C4H5N	1-pentanol	C5H12O	0.798	373.2	2012	zaw	nge	0	-14.9	-12
2-butenal	C4H6O	ethenyl ethanoate	C4H6O2	0.165	328.14	1975	war	sur	0	-2.4	-2.5
2-butenal	C4H6O	1-butanol	C4H10O	0.289	344.78	1970	rum	kul	0	-21.2	-10.6
2-butenal	C4H6O	water	H2O	0.011	370.12	1969	kil	zad	0	5.8	8.7
2-methyl-2-propenoic acid	C4H6O2	2-methylpropanoic acid	C4H8O2	0.842	361.18	1989	li	xin	0	2.5	2.5
methyl propenoate	C4H6O2	1-butanol	C4H10O	0.9	354.53	1976	chu	dan	0	-2	-0.3
ethenyl ethanoate	C4H6O2	methyl methacrylate	C5H8O2	0.946	347.23	1990	wis	tam	0	2.5	2.5
.gamma.-butyrolactone	C4H6O2	water	H2O	0.368	379.07	1989	ram	oda	0	-4.5	1
ethanoic anhydride	C4H6O3	octane	C8H18	0.032	397.7	1995	haa	hei	0	-0.1	0.1
butanenitrile	C4H7N	1-butanol	C4H10O	0.314	288.15	1995	gar	put	0	-37.6	-23.9
butanenitrile	C4H7N	2-methyl-2-propanol	C4H10O	0.304	303.15	1997	gar	san	3	-14.4	-9.8
butanenitrile	C4H7N	2-methyl-1-propanol	C4H10O	0.511	313.15	1997	gar	san	3	-20.4	-11.7
butanenitrile	C4H7N	(RS)-2-butanol	C4H10O	0.916	293.15	1997	gar	san	1	-9.6	-5.6
butanenitrile	C4H7N	benzene	C6H6	0.603	318.15	1995	art	mun	2	-11	-11.1
2-methylpropanal	C4H8O	ethyl ethanoate	C4H8O2	0.832	313.14	1986	she	bau	0	-0.2	-0.2
butanone	C4H8O	butanoic acid	C4H8O2	0.904	352.13	1977	ras	kie	0	3	3.1
tetrahydrofuran	C4H8O	pyrrolidine	C4H9N	0.755	333.35	1990	wu	loc	0	-1.2	-1.7
butanone	C4H8O	2-methyl-2-propanol	C4H10O	0.883	352.1	1969	ren		0	-2.4	1.1
butanone	C4H8O	(RS)-2-butanol	C4H10O	0.443	361.82	1977	sch	qui	0	-4.7	2.7
butanone	C4H8O	3-pentanone	C5H10O	0.903	354.23	1974	glu	tar	0	-0.3	-0.3
butanone	C4H8O	bromobenzene	C6H5Br	0.952	327.14	1988	ram	kri	3	-1	-1
butanal	C4H8O	benzene	C6H6	0.784	313.14	1989	leu	che	0	1.4	1.4
butanone	C4H8O	benzene	C6H6	0.782	333.13	1984	rat	pal	0	-7.4	-7.4
butanone	C4H8O	cyclohexanone	C6H10O	0.735	360.45	2007	pra	su	0	3.5	3.4

tetrahydrofuran	C4H8O	cyclohexanone	C6H10O	0.402	333.13	1984	rat	par	0	-3.4	-3.4
butanone	C4H8O	cyclohexane	C6H12	0.945	293.15	1989	van	koh	0	-7	-7
tetrahydrofuran	C4H8O	cyclohexane	C6H12	0.077	298.14	1975	des	osw	0	-1.7	-1.6
tetrahydrofuran	C4H8O	cyclohexane	C6H12	0.862	339.15	1993	wan		1	-2.1	-2.1
butanone	C4H8O	hexane	C6H14	0.63	338.13	1972	mar	rat	1	-7	-6.7
tetrahydrofuran	C4H8O	3-methylpentane	C6H14	0.652	334	1999	lor	auc	3	-7.1	-7
tetrahydrofuran	C4H8O	hexane	C6H14	0.966	338.42	1980	lam	mat	0	-1.7	-1.7
butanone	C4H8O	1-hexanol	C6H14O	0.703	313.15	1996	gar	san	2	-7	-2.3
tetrahydrofuran	C4H8O	ethyl 1,1-dimethylethyl ether	C6H14O	0.232	322.32	2003	seg	mej	0	-5.3	-5.2
butanone	C4H8O	toluene	C7H8	0.739	329.34	1972	riv		0	-6.9	-6.9
tetrahydrofuran	C4H8O	toluene	C7H8	0.301	336.13	1975	riv		0	-2.2	-2.3
butanone	C4H8O	methoxybenzene	C7H8O	0.065	333.4	1992	yan	bot	0	-11.2	-11.3
ethyloxirane	C4H8O	heptane	C7H16	0.156	313.15	1994	jon	sav	0	-5.3	-4.9
tetrahydrofuran	C4H8O	heptane	C7H16	0.577	313.14	1988	des	osw	0	-7.1	-7.1
butanal	C4H8O	heptane	C7H16	0.127	318.14	1984	eng	san	0	-10.4	-9.8
butanone	C4H8O	2,4,4-trimethyl-1-pentene	C8H16	0.229	313.14	1989	nhu	sve	0	-17	-16.7
butanone	C4H8O	water	H2O	0.189	346.77	1932	hir		0	-31.6	-14.1
butanone	C4H8O	water	H2O	0.662	346.87	1964	alt	mor	0	-13.3	-2.3
butanone	C4H8O	water	H2O	0.86	347.73	1995	moo	och	0	-9.6	-0.3
tetrahydrofuran	C4H8O	water	H2O	0.048	341.34	1973	pin		0	-21.7	-10.7
tetrahydrofuran	C4H8O	water	H2O	0.8	312	2011	mat	kam	0	-18.6	-10.2
1,4-dioxane	C4H8O2	ethyl ethanoate	C4H8O2	0.797	293.14	1966	ste	bit	0	-7.4	-7.4
1,4-dioxane	C4H8O2	2-chlorobutane	C4H9Cl	0.574	352.15	2003	rey	har	0	-9.6	-9.7
ethyl ethanoate	C4H8O2	diethyl ether	C4H10O	0.1	283.09	1926	sch		0	0.6	0.6
ethyl ethanoate	C4H8O2	1-butanol	C4H10O	0.919	351.73	1986	ort	pen	1	-1.3	-0.1
methyl propanoate	C4H8O2	1-butanol	C4H10O	0.033	348.13	1987	fer	ber	0	-9.5	-4.2
1,4-dioxane	C4H8O2	2-methyl-2-propanol	C4H10O	0.952	333.95	2008	red	rao	0	-5.3	-2.2
propyl methanoate	C4H8O2	2-methyl-1-propanol	C4H10O	0.671	357.25	1999	ort	her	0	-8.6	-3.1
1,4-dioxane	C4H8O2	2-methyl-1-propanol	C4H10O	0.922	333.15	2008	red	rao	0	-6.5	-4.6
propyl methanoate	C4H8O2	(RS)-2-butanol	C4H10O	0.224	364.15	1999	gon	ort	0	-7.1	-0.6
1,4-dioxane	C4H8O2	1-butanamine	C4H11N	0.086	298.14	1988	ace	pos	1	0.6	1.2

ethyl ethanoate	C4H8O2	diethylamine	C4H11N	0.223	331.32	1966	eng	bit	0	1.2	0.3
ethyl ethanoate	C4H8O2	diethylamine	C4H11N	0.578	322.53	1966	eng	bit	1	3.1	0.7
ethyl ethanoate	C4H8O2	diethylamine	C4H11N	0.63	320.64	1969	eng	bit	0	3.9	1.3
1,4-dioxane	C4H8O2	cyclopentane	C5H10	0.885	320.28	2005	rom	vil	0	-18.2	-18.4
ethyl ethanoate	C4H8O2	1-chloropentane	C5H11Cl	0.784	353.75	1994	ort	pen	0	-1.1	-1.2
1,4-dioxane	C4H8O2	benzene	C6H6	0.5	298.14	1972	des	osw	0	-9.6	-9.8
ethyl ethanoate	C4H8O2	benzene	C6H6	0.2	273.1	1926	sch		0	-7.3	-7.4
1,4-dioxane	C4H8O2	cyclohexane	C6H12	0.456	313.14	1988	des	osw	0	-3.3	-3.1
ethyl ethanoate	C4H8O2	butyl ethanoate	C6H12O2	0.313	350.11	2013	laa	pok	1	2.3	2.2
ethyl ethanoate	C4H8O2	hexane	C6H14	0.485	338.48	2010	fer	per	0	0.6	0.6
1,4-dioxane	C4H8O2	toluene	C7H8	0.447	298.14	1975	des	osw	0	-7.6	-7.7
ethyl ethanoate	C4H8O2	toluene	C7H8	0.773	354.26	1962	car	kro	0	-2.5	-2.6
ethyl ethanoate	C4H8O2	toluene	C7H8	0.772	323.14	1972	lin	pro	0	14.5	14.5
butanoic acid	C4H8O2	octane	C8H18	0.736	409.62	1976	rad	han	0	28.7	28.2
1,4-dioxane	C4H8O2	water	H2O	0.57	293.14	1940	nii		0	-32.7	-13.2
1,4-dioxane	C4H8O2	water	H2O	0.035	343.13	1977	kor	val	0	-9.6	-4.1
1,4-dioxane	C4H8O2	water	H2O	0.5	353.15	1997	iul	ham	0	-27.5	-11.6
ethyl ethanoate	C4H8O2	water	H2O	0.433	343.63	1985	ouy	wan	1	-21.8	-6.8
sulfolane	C4H8O2S	benzene	C6H6	0.091	348.13	1985	he	wu	0	-2.2	-2.2
sulfolane	C4H8O2S	1,2-dimethylbenzene	C8H10	0.924	373.1	1995	ton	gao	2	-88.3	-94.9
sulfolane	C4H8O2S	ethylbenzene	C8H10	0.087	357.8	2011	jon	maa	0	-7.9	-7.9
sulfolane	C4H8O2S	1,3-dimethylbenzene	C8H10	0.815	373.1	1995	ton	gao	2	-26.2	-29
methyl 2-hydroxypropanoate	C4H8O3	water	H2O	0.309	283.15	2005	san	gme	0	0.4	-0.3
1-bromobutane	C4H9Br	1-butanol	C4H10O	0.806	313.15	2002	gar	mar	0	-4.6	-3.5
1-bromobutane	C4H9Br	2-methyl-2-propanol	C4H10O	0.406	318.15	2002	gar	mar	0	-10.9	-10.3
1-bromobutane	C4H9Br	2-methyl-1-propanol	C4H10O	0.613	308.15	2003	mar	gar	0	-11.8	-10.5
1-bromobutane	C4H9Br	(RS)-2-butanol	C4H10O	0.097	313.15	2003	mar	gar	0	-17.9	-17.4
1-bromobutane	C4H9Br	1-hexanol	C6H14O	0.764	298.15	2003	gar	mar	0	-4.3	-3.3
1-chlorobutane	C4H9Cl	2-methyl-1-propanol	C4H10O	0.158	308.15	2001	gar	mar	0	-32.2	-30.8
1-chlorobutane	C4H9Cl	(RS)-2-butanol	C4H10O	0.753	308.15	2001	gar	mar	0	-4.5	-3.4
1-chlorobutane	C4H9Cl	chlorobenzene	C6H5Cl	0.825	298.16	1983	khu	mut	1	-1.4	-1.5

1-chlorobutane	C4H9Cl	cyclohexane	C6H12	0.26	351.47	2006	hid	dah	0	1.3	1.5
1-chlorobutane	C4H9Cl	hexane	C6H14	0.3	298.15	2009	per	gin	0	-1.4	-1.2
1-chlorobutane	C4H9Cl	1-hexanol	C6H14O	0.22	318.15	2001	mar	gar	0	-25.3	-22.9
2-chlorobutane	C4H9Cl	toluene	C7H8	0.586	323.15	1996	dah	wic	0	-0.1	-0.1
1-chlorobutane	C4H9Cl	heptane	C7H16	0.474	318.14	1981	ash	ver	0	-0.8	-0.6
1-chlorobutane	C4H9Cl	heptane	C7H16	0.356	360.41	2006	hid	dah	0	-0.6	-0.3
1-chlorobutane	C4H9Cl	2,4,4-trimethyl-1-pentene	C8H16	0.852	293.15	1989	nhu	sve	0	-1	-1
1-chlorobutane	C4H9Cl	2,2,4-trimethylpentane	C8H18	0.59	293.15	1989	van	sve	0	-2.4	-2.2
2-chloro-2-methylpropane	C4H9Cl	2,2,4-trimethylpentane	C8H18	0.77	293.15	1988	van	now	0	-1.7	-1.6
tetrahydro-1,4-oxazine	C4H9NO	1-butanol	C4H10O	0.448	363.35	1991	wu	loc	0	5.8	4.4
2-butanone oxime	C4H9NO	3-pentanone	C5H10O	0.954	353.13	1968	gei	koe	0	-22.9	-19.1
tetrahydro-1,4-oxazine	C4H9NO	cyclohexane	C6H12	0.673	364.24	2010	mar	san	0	2.4	-1.6
2-butanone oxime	C4H9NO	heptane	C7H16	0.895	338.13	1968	gei	koe	0	3.1	1.7
1-butanol	C4H10O	2-methyl-2-propanol	C4H10O	0.7	329.65	1969	qui	koe	0	7.6	7.6
1-butanol	C4H10O	2-methyl-1-propanol	C4H10O	0.182	382.22	1975	tam	wis	0	-1.2	-1.2
1-butanol	C4H10O	(RS)-2-butanol	C4H10O	0.128	313.14	1973	gei	sue	0	-2.5	-2.5
2-methyl-1-propanol	C4H10O	(RS)-2-butanol	C4H10O	0.647	377.92	1975	wis	tam	1	1	1
1-butanol	C4H10O	3-oxa-1,5-pentanediol	C4H10O3	0.8	351.13	1977	vis	evd	1	0.5	0.6
2-methyl-2-propanol	C4H10O	pyridine	C5H5N	0.597	313.14	1977	war		1	2.2	8.1
(RS)-2-butanol	C4H10O	2,4-pentanedione	C5H8O2	0.509	298.14	1980	kat		0	-16.1	-5.6
2-methyl-1-propanol	C4H10O	tetrahydropyran	C5H10O	0.199	344.3	2008	uno	mat	0	-5.1	-1.7
(RS)-2-butanol	C4H10O	tetrahydropyran	C5H10O	0.495	353.41	2008	uno	mat	0	-9	-1.9
1-butanol	C4H10O	propyl ethanoate	C5H10O2	0.691	381.97	1987	ort	oco	0	-9.2	-1.6
1-butanol	C4H10O	methyl butanoate	C5H10O2	0.609	368.13	1987	fer	ber	0	-11	-2.8
(RS)-2-butanol	C4H10O	propyl ethanoate	C5H10O2	0.688	361.93	1999	gon	ort	0	-47	-38.8
(RS)-2-butanol	C4H10O	butyl methanoate	C5H10O2	0.757	371.02	1996	gon	ort	2	-6.2	-2
1-butanol	C4H10O	diethyl carbonate	C5H10O3	0.832	389.67	2003	rod	can	2	-5.8	-2.1
1-butanol	C4H10O	2-methyl-2-butanol	C5H12O	0.395	380.12	1976	and	kom	0	-1.6	-1.6
2-methyl-2-propanol	C4H10O	1-pentanol	C5H12O	0.131	313.14	1989	ora		0	9.6	9.5
2-methyl-2-propanol	C4H10O	1,1-dimethylethyl methyl ether	C5H12O	0.512	336.95	1999	lor	auc	1	-13.3	-5.2

1-butanol	C4H10O	bromobenzene	C6H5Br	0.854	367.14	1997	art	laf	0	-3.1	-2.7
2-methyl-2-propanol	C4H10O	bromobenzene	C6H5Br	0.608	362.27	2001	art	laf	1	-9.5	-9.1
1-butanol	C4H10O	chlorobenzene	C6H5Cl	0.192	364.55	1997	art	laf	0	-6.8	-4.8
2-methyl-2-propanol	C4H10O	chlorobenzene	C6H5Cl	0.237	344.05	2001	art	laf	1	-17.7	-15.9
1-butanol	C4H10O	2-chlorophenol	C6H5ClO	0.456	383.15	1995	gab	mar	0	-7.7	-13.2
diethyl ether	C4H10O	benzene	C6H6	0.285	293.14	1938	tah		0	-4.4	-4.2
1-butanol	C4H10O	benzene	C6H6	0.176	313.14	1980	ora	kol	0	-3.4	-2.3
2-methyl-2-propanol	C4H10O	benzene	C6H6	0.857	343.13	1973	rui		0	-8.2	-7.4
2-methyl-1-propanol	C4H10O	benzene	C6H6	0.095	352.92	1967	nat	rao	0	-0.3	0.8
2-methyl-1-propanol	C4H10O	benzene	C6H6	0.256	308.15	1998	bha	mak	1	-11.9	-10.5
(RS)-2-butanol	C4H10O	benzene	C6H6	0.941	313.15	2006	vil	mar	0	-20.3	-19.2
2-methyl-1-propanol	C4H10O	cyclohexanone	C6H10O	0.602	389.45	2007	pra	sud	0	-2.9	1.8
1-butanol	C4H10O	cyclohexane	C6H12	0.758	363.02	1963	rao	rao	4	-12.9	-12.6
1-butanol	C4H10O	cyclohexane	C6H12	0.703	359.79	1983	zon	yan	0	-14.3	-14
2-methyl-2-propanol	C4H10O	cyclohexane	C6H12	0.229	324.2	1969	ren		0	-2.5	-2.4
(RS)-2-butanol	C4H10O	cyclohexane	C6H12	0.689	313.15	2009	gie	kos	0	-7.5	-7.7
1-butanol	C4H10O	butyl ethanoate	C6H12O2	0.261	393.47	1987	ort	pen	0	-6	0.5
2-methyl-2-propanol	C4H10O	propyl propanoate	C6H12O2	0.589	363.41	2006	ort	esp	0	-3.1	1.3
2-methyl-2-propanol	C4H10O	1,1-dimethylethyl ethanoate	C6H12O2	0.672	357.5	2005	mon	mun	0	-1.1	3.2
2-methyl-1-propanol	C4H10O	propyl propanoate	C6H12O2	0.15	390.7	1999	ort	her	0	-2.8	2.8
(RS)-2-butanol	C4H10O	1-methylpropyl ethanoate	C6H12O2	0.574	374.95	2013	wan	xia	0	0.8	6.4
1-butanol	C4H10O	2-methylpentane	C6H14	0.136	303.15	1994	gar	san	0	-2.5	-2.2
1-butanol	C4H10O	hexane	C6H14	0.427	323.12	1992	gra	gar	0	-7.8	-7.4
1-butanol	C4H10O	hexane	C6H14	0.982	293.12	1992	gra	san	0	-36.3	-37.5
1-butanol	C4H10O	2,3-dimethylbutane	C6H14	0.511	298.15	1994	gar	per	0	-12.3	-12.2
2-methyl-2-propanol	C4H10O	hexane	C6H14	0.696	298.15	1993	rod	par	0	-1.8	-2.3
(RS)-2-butanol	C4H10O	hexane	C6H14	0.13	323.15	1993	ara	mac	0	-5.6	-5.1
1-butanol	C4H10O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.048	313.15	2006	vil	mar	1	-0.8	-0.4
1-butanol	C4H10O	dipropyl ether	C6H14O	0.803	323.15	1997	gar	per	0	-33	-21.8
2-methyl-1-propanol	C4H10O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.6	313.15	2006	vil	cha	0	-40	-24.2

2-methyl-1-propanol	C4H10O	dipropyl ether	C6H14O	0.4	308.15	1998	gar	san	0	-18.2	-10.8
(RS)-2-butanol	C4H10O	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.499	313.15	2006	vil	mar	0	-31.1	-19.9
(RS)-2-butanol	C4H10O	dipropyl ether	C6H14O	0.617	313.15	1998	gar	san	0	-24.2	-15.8
(RS)-2-butanol	C4H10O	1-propoxy-2-propanol	C6H14O2	0.767	339.4	2008	ram	neu	0	-1.2	-1.1
1-butanol	C4H10O	triethylamine	C6H15N	0.491	313.14	1975	chu	dru	0	-5.1	4.2
2-methyl-2-propanol	C4H10O	triethylamine	C6H15N	0.129	303.19	1975	chu	dru	0	-7.5	-3
1-butanol	C4H10O	toluene	C7H8	0.204	333.29	1977	lne	wic	0	-6.3	-4.9
1-butanol	C4H10O	toluene	C7H8	0.503	368	1997	dar	alk	0	-6.2	-4.4
2-methyl-1-propanol	C4H10O	toluene	C7H8	0.407	343.38	1977	lne	wic	0	-9.9	-8.3
(RS)-2-butanol	C4H10O	toluene	C7H8	0.887	308.15	2004	mak	bha	0	-16.9	-16.3
2-methyl-1-propanol	C4H10O	2-methylphenol	C7H8O	0.793	386.85	2006	pra	jai	0	2.4	1.8
2-methyl-2-propanol	C4H10O	methylcyclohexane	C7H14	0.979	355.3	1999	mar	pen	0	0.7	0.7
1-butanol	C4H10O	heptane	C7H16	0.746	338.13	1980	kum	kat	0	-28	-27.9
1-butanol	C4H10O	heptane	C7H16	0.892	360.95	2010	moh	mem	0	-8.8	-8.6
2-methyl-2-propanol	C4H10O	heptane	C7H16	0.602	338.13	1980	kum	kat	0	-2.5	-2.5
2-methyl-1-propanol	C4H10O	heptane	C7H16	0.551	348.13	1980	kum	kat	1	-11.2	-10.7
(RS)-2-butanol	C4H10O	heptane	C7H16	0.925	348.13	1980	kum	kat	1	-4.4	-4.4
(RS)-2-butanol	C4H10O	1,1-dimethylpropyl ethyl ether	C7H16O	0.09	358.06	2012	sun	laa	0	-9.3	-5.8
1-butanol	C4H10O	ethylbenzene	C8H10	0.907	309.94	1977	mat	mun	0	-13.4	-13
2-methyl-2-propanol	C4H10O	2,4,4-trimethyl-1-pentene	C8H16	0.404	333.14	2007	mal		0	-4.1	-3.7
(RS)-2-butanol	C4H10O	2,4,4-trimethyl-1-pentene	C8H16	0.179	360.17	2001	uus	pok	0	-3.2	-2
1-butanol	C4H10O	octane	C8H18	0.273	288.18	1992	gra	gar	1	-8.2	-8.2
2-methyl-1-propanol	C4H10O	2,2,4-trimethylpentane	C8H18	0.941	348.15	2011	ber	pav	1	-10	-9.9
diethyl ether	C4H10O	water	H2O	0.01	298.14	1969	sig	arm	0	49.2	51.9
1-butanol	C4H10O	water	H2O	0.812	374.32	1960	orr	coa	0	0.4	-4.3
1-butanol	C4H10O	water	H2O	0.95	333.13	1971	sch	sch	0	-11.5	-15.8
2-methyl-2-propanol	C4H10O	water	H2O	0.032	343.13	1968	qui	kop	0	9.2	-1.3
2-methyl-2-propanol	C4H10O	water	H2O	0.038	303.15	1990	kog	won	0	27.1	17
2-methyl-2-propanol	C4H10O	water	H2O	0.07	355.49	2002	yan	wan	0	18.7	11
(RS)-2-butanol	C4H10O	water	H2O	0.017	364.12	1942	boe	han	0	11.7	5.9

(RS)-2-butanol	C4H10O	water	H2O	0.027	361.59	1964	alt	bel	0	10.4	3.8
(RS)-2-butanol	C4H10O	water	H2O	0.7	298.14	1987	gau	kre	0	6.6	0.8
2-ethoxyethanol	C4H10O2	butyl methanoate	C5H10O2	0.314	333.15	2004	chy	fra	0	-13.2	-10.4
2-ethoxyethanol	C4H10O2	phenol	C6H6O	0.171	363.15	2001	chy	fra	0	1.8	-2.9
2-ethoxyethanol	C4H10O2	cyclohexane	C6H12	0.601	303.15	2000	car	gon	0	-18.6	-19.4
1-methoxy-2-propanol	C4H10O2	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.2	340	2004	psu	wic	0	-6.3	-4.6
2-ethoxyethanol	C4H10O2	benzene, ethenyl-	C8H8	0.46	334.63	1968	gar	bov	0	9.1	9.5
2-ethoxyethanol	C4H10O2	1,2-dimethylbenzene	C8H10	0.181	338.13	1968	gar	bov	0	17.8	18.1
2-ethoxyethanol	C4H10O2	octane	C8H18	0.349	390.18	1957	mur	van	0	-3.1	-3
2-ethoxyethanol	C4H10O2	water	H2O	0.161	371.32	1956	bou	kuc	0	3.7	2.3
1-butanamine	C4H11N	piperidine	C5H11N	0.324	343.15	2000	bel	bel	0	-0.7	-0.3
2-methyl-2-propanamine	C4H11N	hexane	C6H14	0.486	323.15	1995	wol	lan	0	9.2	6.4
1-butanamine	C4H11N	hexane	C6H14	0.289	283.15	1995	wol	lan	0	6.1	2.3
diethylamine	C4H11N	hexane	C6H14	0.593	313.14	1985	wol	sch	0	4.9	3.1
N-deuterodiethylamine	C4H11N	hexane	C6H14	0.561	333.13	1985	wol	sch	0	5.2	3.2
diethylamine	C4H11N	triethylamine	C6H15N	0.7	323.13	1962	bit	kau	0	1.2	1.1
2-amino-2-methyl-1-propanol	C4H11NO	water	H2O	0.251	377.75	2006	pap	ana	0	11.9	10.2
bis(2-hydroxyethyl)amine	C4H11NO2	water	H2O	0.271	365.15	2002	hor	mou	0	17.2	14.2
1,4-butanediamine	C4H12N2	water	H2O	0.498	363.15	2011	ahm	neg	0	50.2	42.3
tetramethylsilane	C4H12Si	2,2-dimethylpropane	C5H12	0.242	263.2	1970	hoe	kre	0	0.5	0.5
2-furaldehyde	C5H4O2	2-methylfuran	C5H6O	0.185	298.74	1946	hol	hix	0	-6.5	-6.5
2-furaldehyde	C5H4O2	4-methyl-2-pentanone	C6H12O	0.856	368.07	1987	hau	wu	0	-6.2	-6.3
2-furaldehyde	C5H4O2	toluene	C7H8	0.411	361.03	1973	riv		0	-7.3	-7.2
2-furaldehyde	C5H4O2	toluene	C7H8	0.701	357.83	1973	riv		1	-13.8	-13.7
2-furaldehyde	C5H4O2	water	H2O	0.949	323.14	1970	kha	per	0	14.1	46.1
pyridine	C5H5N	benzene	C6H6	0.031	298.14	1970	kor	sha	0	-0.7	-0.7
pyridine	C5H5N	3-methylpyridine	C6H7N	0.36	402.42	1978	byk	gus	0	-4.8	-4.8
pyridine	C5H5N	cyclohexane	C6H12	0.284	308.14	1973	ani	kon	0	-2.7	-2.3
pyridine	C5H5N	toluene	C7H8	0.705	303.14	1973	ani	kon	0	-3.6	-3.6
pyridine	C5H5N	toluene	C7H8	0.756	333.13	1988	jos	mic	0	-2.6	-2.6

pyridine	C5H5N	heptane	C7H16	0.438	353.12	1963	mac		1	-4.6	-4
pyridine	C5H5N	octane	C8H18	0.437	353.12	1963	mac	zie	1	-5.4	-4.8
pyridine	C5H5N	2,2,4-trimethylpentane	C8H18	0.503	298.14	1973	ani	kon	0	-14.1	-13.5
pyridine	C5H5N	water	H2O	0.041	324.43	1952	fow		0	9	13.5
pyridine	C5H5N	water	H2O	0.216	321.93	1965	woy	kur	0	8.9	14.2
pyridine	C5H5N	water	H2O	0.852	378.8	1998	dha	raj	0	6.2	19.7
3-methylthiophene	C5H6S	hexane	C6H14	0.73	333.15	2010	sap	uus	0	-5.3	-4.8
3-methylthiophene	C5H6S	toluene	C7H8	0.805	387.21	2012	guo	bai	0	-1.1	-1.1
2-methyl-1,3-butadiene	C5H8	2-methyl-1-butene	C5H10	0.3	310.92	1981	sha	how	0	0	0.1
2-methyl-1,3-butadiene	C5H8	pentane	C5H12	0.798	313.13	1985	how	swi	1	3.1	3.2
cyclopentanone	C5H8O	3-methyl-1-butanol	C5H12O	0.605	402.17	1992	kat	mar	1	-6.6	-0.4
methyl methacrylate	C5H8O2	cyclohexane	C6H12	0.855	318.11	1984	hul	lu	0	4.4	4.3
N-methyl-2-pyrrolidone	C5H9NO	benzene	C6H6	0.955	350	1996	lin	wic	1	-26.2	-27
N-methyl-2-pyrrolidone	C5H9NO	cyclohexane	C6H12	0.66	333.23	1985	gie	rog	0	-48.5	-48.2
N-methyl-2-pyrrolidone	C5H9NO	toluene	C7H8	0.382	383.32	1985	gie	rog	0	-12	-12.2
N-methyl-2-pyrrolidone	C5H9NO	heptane	C7H16	0.024	298.14	1987	gau	kre	0	-0.7	-0.7
N-methyl-2-pyrrolidone	C5H9NO	water	H2O	0.043	380.24	1996	nol	fis	0	0.9	1
N-formylmorpholine	C5H9NO2	heptane	C7H16	0.358	343.15	2013	moo	nai	0	0.5	1.1
tetrahydropyran	C5H10O	piperidine	C5H11N	0.06	323.15	1992	ait	bel	0	-1.7	-1.7
pentanal	C5H10O	benzene	C6H6	0.143	313.14	1986	kas	kna	1	-1.3	-1.3
tetrahydropyran	C5H10O	aniline	C6H7N	0.248	308.15	2010	jan	yad	0	-57.2	16.3
2-methyltetrahydrofuran	C5H10O	cyclohexane	C6H12	0.86	310.95	1999	hor	gar	0	-1.4	-1.4
3-methyl-2-butanone	C5H10O	2,3-dimethylbutane	C6H14	0.792	333.15	2013	pav	and	0	-14.4	-14.2
3-pentanone	C5H10O	hexane	C6H14	0.18	325.14	1979	bar	dia	0	10.7	10.8
3-methyl-2-butanone	C5H10O	2-methylpentane	C6H14	0.393	330	2005	psu	wic	1	-8.5	-8.3
tetrahydropyran	C5H10O	hexane	C6H14	0.074	333.13	2012	mej	seg	1	-0.6	-0.6
2-methylpropyl methanoate	C5H10O2	butyl methanoate	C5H10O2	0.374	375.2	1985	ses	mir	0	-2.8	-2.8
propyl ethanoate	C5H10O2	benzene	C6H6	0.605	365.23	1972	fah	elg	0	-1.7	-1.7
propyl ethanoate	C5H10O2	2-hexyne	C6H10	0.328	363.15	2010	neg	kac	0	-2.2	-2.3
1-methylethyl ethanoate	C5H10O2	cyclohexane	C6H12	0.149	348.14	1994	kri	vis	0	1.4	1.5
propyl ethanoate	C5H10O2	cyclohexane	C6H12	0.644	293.15	2007	neg	bel	0	-0.7	-0.7

propyl ethanoate	C5H10O2	1-hexene	C6H12	0.668	303.15	2007	neg	bel	0	-2.8	-2.9
propyl ethanoate	C5H10O2	heptane	C7H16	0.988	373.72	2001	ort	gon	0	-0.7	-0.7
methyl butanoate	C5H10O2	heptane	C7H16	0.876	371.35	2012	rio	ort	0	0.1	0.1
furfuryl alcohol, tetrahydro-	C5H10O2	water	H2O	0.173	326.34	1971	tsi	vas	1	4.3	2.9
diethyl carbonate	C5H10O3	1,1-dimethylethyl methyl ether	C5H12O	0.555	298.15	1997	fra	com	2	-4.4	-4.5
1-chloropentane	C5H11Cl	hexane	C6H14	0.821	288.15	2009	per	gin	0	-4.4	-4
piperidine	C5H11N	N-propyl-1-propanamine	C6H15N	0.562	333.15	2000	bel	bel	0	-2	-2.2
N-methylmorpholine	C5H11NO	water	H2O	0.349	333.15	2009	bel	raz	0	8.5	15.4
pentane	C5H12	benzene	C6H6	0.161	308.14	1971	wan	lu	0	0.2	1.1
2,2-dimethylpropane	C5H12	benzene	C6H6	0.114	273.2	1953	mat	des	0	-26.4	-24.7
pentane	C5H12	methylcyclopentane	C6H12	0.874	311.88	1957	mye		1	-0.3	-0.3
pentane	C5H12	hexane	C6H14	0.668	298.14	1974	che	zwo	0	1.4	1.4
pentane	C5H12	toluene	C7H8	0.14	303.34	1972	li	won	0	-3.1	-2.3
2-methyl-2-butanol	C5H12O	2-methyl-1-butanol	C5H12O	0.126	373.15	1994	auc	bur	2	-1.7	-1.8
2-methyl-2-butanol	C5H12O	benzene	C6H6	0.802	313.15	2001	rho	gri	0	-15.6	-13.8
1-pentanol	C5H12O	aniline	C6H7N	0.407	373.12	1974	sur	doj	0	-27	-33.9
1,1-dimethylethyl methyl ether	C5H12O	2-hexyne	C6H10	0.572	273.34	2006	bou	bel	0	-2	-2
1-pentanol	C5H12O	cyclohexane	C6H12	0.6	328.24	1973	min	rue	0	4.6	4.8
1,1-dimethylethyl methyl ether	C5H12O	cyclohexane	C6H12	0.401	308.15	2001	del	hor	0	0.3	0.3
2-pentanol	C5H12O	cyclohexane	C6H12	0.466	353.15	2009	gie	kos	0	-2.2	-1.7
1,1-dimethylethyl methyl ether	C5H12O	1-hexene	C6H12	0.149	313.15	1998	seg	mar	2	-0.6	-0.6
butyl methyl ether	C5H12O	1-hexene	C6H12	0.802	303.15	2012	han	sol	0	-5.5	-5.5
2-methyl-2-butanol	C5H12O	hexane	C6H14	0.981	338.15	2010	gie	kos	1	-5.3	-5.4
1,1-dimethylethyl methyl ether	C5H12O	hexane	C6H14	0.82	328	1979	plu	mat	0	0.9	0.9
1,1-dimethylethyl methyl ether	C5H12O	1-hexanol	C6H14O	0.781	318.15	2003	jim	seg	0	-4.2	-1.2
1-pentanol	C5H12O	toluene	C7H8	0.25	363.13	1971	sad	luf	0	0	1.6
1-pentanol	C5H12O	methylcyclohexane	C7H14	0.437	313.14	1980	ora		0	-7.9	-7.6
1,1-dimethylethyl methyl ether	C5H12O	1-heptene	C7H14	0.99	311.15	1993	ben	lam	0	2.6	2.6
1-pentanol	C5H12O	heptane	C7H16	0.848	363.25	1979	tre	tre	0	-4.8	-4.3
3-methyl-1-butanol	C5H12O	heptane	C7H16	0.077	358.13	1988	mac	lin	0	-1.1	-0.5

2-methyl-1-butanol	C5H12O	heptane	C7H16	0.569	358.15	1991	wol	lin	0	-8.9	-8.1
1,1-dimethylethyl methyl ether	C5H12O	heptane	C7H16	0.43	298.15	1997	moe	cot	0	4.5	4.6
3-pentanol	C5H12O	heptane	C7H16	0.187	368.15	1990	wol	lin	0	0.9	1.7
3-methyl-2-butanol	C5H12O	heptane	C7H16	0.5	313.15	1997	rho	bhe	0	-6	-5.7
1-pentanol	C5H12O	1,4-dimethylbenzene	C8H10	0.883	408.24	1967	gal		3	-0.9	-0.1
1-pentanol	C5H12O	2,2,4-trimethylpentane	C8H18	0.148	313.15	2013	mor	mar	0	-2.6	-2.1
1,1-dimethylethyl methyl ether	C5H12O	2,2,4-trimethylpentane	C8H18	0.317	339.28	2001	ber	wic	0	6	6.1
2-methyl-2-butanol	C5H12O	water	H2O	0.415	283.3	1996	fis	shu	0	9.2	4.4
2-methyl-2-butanol	C5H12O	water	H2O	0.488	343.25	1996	fis	shu	0	5.2	1.2
N-methyldiethanolamine	C5H13NO2	water	H2O	0.444	333.8	2010	del	uus	1	22.8	13.2
bromobenzene	C6H5Br	nitrobenzene	C6H5NO2	0.532	440.91	1985	red	rao	3	-2.8	-3.5
chlorobenzene	C6H5Cl	benzene	C6H6	0.078	356.45	2001	rol	kra	0	3.3	3.3
chlorobenzene	C6H5Cl	aniline	C6H7N	0.388	298.14	1967	des	pan	0	13.6	7.1
chlorobenzene	C6H5Cl	cyclohexane	C6H12	0.346	363.23	1976	rao	rao	1	2.7	2.9
chlorobenzene	C6H5Cl	toluene	C7H8	0.215	303.14	1972	kho	mah	1	-1.6	-1.6
chlorobenzene	C6H5Cl	methylcyclohexane	C7H14	0.932	348.13	1980	dia	cre	0	0.5	0.7
chlorobenzene	C6H5Cl	heptane	C7H16	0.752	353.13	1971	let	bay	0	-2.1	-1.6
chlorobenzene	C6H5Cl	ethylbenzene	C8H10	0.599	293.15	1979	mah	smi	0	-1.5	-1.6
fluorobenzene	C6H5F	cyclohexane	C6H12	0.544	348.13	1980	dia	com	1	-0.2	0.2
fluorobenzene	C6H5F	toluene	C7H8	0.891	333.36	1968	bha	muk	0	-0.1	-0.1
fluorobenzene	C6H5F	methylcyclohexane	C7H14	0.462	333.17	1968	bha	muk	0	0.6	1
nitrobenzene	C6H5NO2	aniline	C6H7N	0.05	342.82	1955	hol	rig	0	0.6	1.2
nitrobenzene	C6H5NO2	1-heptanol	C7H16O	0.479	450.15	2013	mam	tas	0	-16.4	-13
benzene	C6H6	cyclohexane	C6H12	0.899	352.14	1950	sie		0	2.2	2.4
benzene	C6H6	cyclohexane	C6H12	0.101	318.13	1966	mad	mur	0	-42.6	-42.2
benzene	C6H6	cyclohexane	C6H12	0.265	295.51	1973	li	lu	0	2.3	2.8
benzene	C6H6	cyclohexane	C6H12	0.663	254.63	1974	jac		2	2.3	2.9
benzene	C6H6	cyclohexane	C6H12	0.623	313.09	1982	men	gre	0	4.2	4.7
benzene	C6H6	cyclohexane	C6H12	0.276	343.13	1995	lee	hu	0	2.6	3
benzene	C6H6	cyclohexane	C6H12	0.579	350.6	2001	rol	kra	0	4	4.4
benzene	C6H6	cyclohexane	C6H12	0.498	343.03	2007	uno	kur	0	4.1	4.5

benzene	C6H6	1-hexene	C6H12	0.298	312.35	2002	cha	seg	2	-4.6	-4.4
benzene	C6H6	methylcyclopentane	C6H12	0.699	347.74	1962	sus	lyz	0	3.6	4
benzene	C6H6	2-methylpentane	C6H14	0.675	303.14	1972	fun	cha	0	-3.3	-2.6
benzene	C6H6	hexane	C6H14	0.61	344.67	1955	mye		0	2.3	2.8
benzene	C6H6	hexane	C6H14	0.294	328.23	1963	ho	lu	0	1.1	1.5
benzene	C6H6	hexane	C6H14	0.846	303.14	1972	li	won	0	1.4	2
benzene	C6H6	hexane	C6H14	0.256	298.14	1975	mur	mar	0	1.3	1.7
benzene	C6H6	hexane	C6H14	0.138	298.12	1999	wu	li	0	1	1.3
benzene	C6H6	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.298	313.15	2006	vil	mar	0	-4.4	-4.2
benzene	C6H6	dipropyl ether	C6H14O	0.478	333.13	1972	lin	wic	0	-0.4	-0.1
benzene	C6H6	benzonitrile	C7H5N	0.586	323.15	1999	hor	gar	2	-3.9	-3.9
benzene	C6H6	toluene	C7H8	0.9	333.12	1926	sch		0	-2.7	-2.7
benzene	C6H6	toluene	C7H8	0.719	359.65	1993	jin	hu	1	0.7	0.7
benzene	C6H6	methoxybenzene	C7H8O	0.914	342.75	1995	vis	rao	2	0.1	0.1
benzene	C6H6	methylcyclohexane	C7H14	0.938	313.14	1980	asm	gor	0	0.8	0.9
benzene	C6H6	2,4-dimethylpentane	C7H16	0.631	349.92	1962	ste	van	0	0.3	0.8
benzene	C6H6	heptane	C7H16	0.299	362.22	1950	sie		0	3.7	4.2
benzene	C6H6	heptane	C7H16	0.9	312.93	1959	nie	web	0	0.5	0.7
benzene	C6H6	heptane	C7H16	0.21	328.14	1971	kud	vii	0	-0.3	0.3
benzene	C6H6	heptane	C7H16	0.1	359.93	1975	tri	ass	0	2.1	2.4
benzene	C6H6	heptane	C7H16	0.299	313.15	2002	cha	seg	1	3.3	3.9
benzene	C6H6	2,3-dimethylpentane	C7H16	0.373	355.92	1960	kyl	tet	0	2	2.4
benzene	C6H6	octane	C8H18	0.078	313.15	1994	gor		0	5.9	6.6
phenol	C6H6O	2-methylphenol	C7H8O	0.821	457.05	1917	fox	bar	0	2.1	2.1
phenol	C6H6O	4-methylphenol	C7H8O	0.118	428.35	1992	sel	dut	0	2.1	2.1
phenol	C6H6O	3-methylphenol	C7H8O	0.049	409.42	1989	cep	gon	0	-2.6	-2.6
aniline	C6H7N	cyclohexane	C6H12	0.061	323.34	1968	abe	ser	0	1.3	0.7
aniline	C6H7N	hexane	C6H14	0.946	338.13	1968	cam	kar	0	-28.4	-32.5
2-methylpyridine	C6H7N	toluene	C7H8	0.492	313.15	1993	war		0	-2.4	-2.4
aniline	C6H7N	3-methylphenol	C7H8O	0.596	437.81	1985	kre	mai	0	3	-1.4

aniline	C6H7N	benzene, ethenyl-	C8H8	0.652	363.13	1985	gme		0	3.3	-3.2
aniline	C6H7N	2,2,4-trimethylpentane	C8H18	0.587	353.16	1958	zie		1	2.3	-1.4
4-methylpyridine	C6H7N	water	H2O	0.06	370.48	1958	zie	mac	1	5.8	8.4
2-methylpyridine	C6H7N	water	H2O	0.039	368.02	1953	vri	med	0	12.2	16.1
cyclohexene	C6H10	cyclohexane	C6H12	0.79	355.5	2004	ste	sun	0	1.1	1.1
3-hexyne	C6H10	octane	C8H18	0.764	298.15	2000	bou	bel	0	0.6	0.7
cyclohexanone	C6H10O	cyclohexanol	C6H12O	0.804	338.57	1963	eng	bit	0	1.9	5.2
cyclohexanone	C6H10O	cyclohexanol	C6H12O	0.74	323.15	2008	abb	gme	0	-8.6	-4
cyclohexanone	C6H10O	water	H2O	0.01	363.12	1959	gor	mor	0	-7.8	-6.5
1-aza-2-cycloheptanone	C6H11NO	water	H2O	0.137	308.19	1969	sus	ard	0	4.1	2.7
methylcyclopentane	C6H12	cyclohexane	C6H12	0.477	349.3	1970	wea	van	0	0.3	0.3
cyclohexane	C6H12	4-methyl-2-pentanone	C6H12O	0.963	353.6	2010	mar	lor	1	-0.9	-0.8
cyclohexane	C6H12	butyl ethanoate	C6H12O2	0.058	354.85	2012	li	li	0	4.8	4.8
cyclohexane	C6H12	cyclohexaneamine	C6H13N	0.707	313.14	1968	ker	ser	0	8.5	5.5
cyclohexane	C6H12	1H-azepine, hexahydro-	C6H13N	0.04	298.14	1973	cab	cec	0	7.8	6
cyclohexane	C6H12	hexane	C6H14	0.409	346.02	1967	rid	but	0	-0.3	-0.3
cyclohexane	C6H12	hexane	C6H14	0.203	293.15	2000	gor	ora	0	-1.4	-1.4
1-hexene	C6H12	hexane	C6H14	0.069	325.6	2009	mar	auc	0	0.3	0.3
cyclohexane	C6H12	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.132	342.55	1995	wis		0	0.5	0.5
1-hexene	C6H12	1-hexanamine	C6H15N	0.11	333.12	1967	hum	van	0	9	1.5
cyclohexane	C6H12	toluene	C7H8	0.81	357.04	1950	sie		0	1.2	1.4
cyclohexane	C6H12	toluene	C7H8	0.309	339.43	1969	riv		0	3.5	3.9
cyclohexane	C6H12	toluene	C7H8	0.666	359.8	1981	cho	pal	0	2.4	2.6
cyclohexane	C6H12	heptane	C7H16	0.22	366.67	1957	mye		1	-1.3	-1.3
cyclohexane	C6H12	heptane	C7H16	0.8	313.15	1995	loz	mon	0	-1	-1
cyclohexane	C6H12	ethylbenzene	C8H10	0.715	323.14	1974	jai	yad	1	-1.4	-1.3
cyclohexane	C6H12	2,2,4-trimethylpentane	C8H18	0.712	308.14	1974	jai	yad	0	-3.3	-3.3
cyclohexanol	C6H12O	butyl ethanoate	C6H12O2	0.3	404.12	1968	nag	men	0	-1.9	2.2
2-hexanone	C6H12O	methoxybenzene	C7H8O	0.218	410.82	2009	kir	kuu	0	-0.7	-0.7
cyclohexanol	C6H12O	1,4-dimethylbenzene	C8H10	0.727	339.13	1988	com	fra	0	-15.4	-13.3

cyclohexanol	C6H12O	1,3-dimethylbenzene	C8H10	0.031	360.6	2002	swi	mal	0	0.6	1.3
4-methyl-2-pentanone	C6H12O	octane	C8H18	0.721	384	1999	wis		0	-4.3	-4.1
4-methyl-2-pentanone	C6H12O	2,2,4-trimethylpentane	C8H18	0.763	333.15	2011	ber	pav	1	-9.3	-9.1
butyl ethanoate	C6H12O2	toluene	C7H8	0.856	395.12	1968	mai	men	0	-0.8	-0.9
ethyl butanoate	C6H12O2	heptane	C7H16	0.459	376.42	2012	rio	ort	0	2.2	2.3
2-methylpropyl ethanoate	C6H12O2	heptane	C7H16	0.282	372.8	1991	mat	bon	0	2.2	2.3
1H-azepine, hexahydro-	C6H13N	1,6-hexanediamine	C6H16N2	0.5	373.12	1965	dei	kog	0	6.4	5.9
2-methylpentane	C6H14	hexane	C6H14	0.899	313.14	1979	ho	dav	0	-0.4	-0.4
hexane	C6H14	1-hexanol	C6H14O	0.806	333.15	1978	wie	ste	0	-1.8	-1.2
hexane	C6H14	methoxybenzene	C7H8O	0.693	333.17	1992	yan	bot	0	-0.2	0
hexane	C6H14	2,6-dimethylpyridine	C7H9N	0.876	263.15	2005	ben	ait	0	-10.5	-10.4
3-methylpentane	C6H14	heptane	C7H16	0.658	328.15	1994	ber	lai	0	0.5	0.5
hexane	C6H14	octane	C8H18	0.125	298.15	1990	she	anx	0	-0.6	-0.6
1,4-dimethylpiperazine	C6H14N2	heptane	C7H16	0.141	273.15	1997	dah	kac	0	0.4	0.5
4-methyl-2-pentanol	C6H14O	toluene	C7H8	0.089	343.13	1974	gop	dak	0	-11.1	-10
1-methyl-1-(1-methylethoxy)ethane	C6H14O	toluene	C7H8	0.642	343.15	2007	did	ait	0	-5	-4.9
1-methyl-1-(1-methylethoxy)ethane	C6H14O	heptane	C7H16	0.449	313.15	2002	cha	seg	0	3	3.1
ethyl 1,1-dimethylethyl ether	C6H14O	heptane	C7H16	0.783	328.15	2001	del	hor	0	1.5	1.5
1-methyl-1-(1-methylethoxy)ethane	C6H14O	1,3-dimethylbenzene	C8H10	0.057	273.15	2007	did	ait	0	-49.1	-48.7
1-methyl-1-(1-methylethoxy)ethane	C6H14O	water	H2O	0.1	335.32	1967	yor	yos	0	45.9	51.3
2-butoxyethanol	C6H14O2	ethylcyclohexane	C8H16	0.064	382.73	1963	pra	van	1	0.4	0.7
triethylamine	C6H15N	water	H2O	0.503	284.14	1907	lat		0	-0.9	4.4
triethylamine	C6H15N	water	H2O	0.043	295.14	1960	kri	kha	1	-29.1	-17.3
benzonitrile	C7H5N	toluene	C7H8	0.987	353.15	1999	hor	gar	2	-4.3	-4.2
benzaldehyde	C7H6O	toluene	C7H8	0.3	372.97	1972	pav	pop	0	4.1	4.1
benzaldehyde	C7H6O	2-methylphenol	C7H8O	0.849	340.13	1980	vos	kom	1	19.7	20.8
2-chlorotoluene	C7H7Cl	4-chlorotoluene	C7H7Cl	0.771	373.15	1992	bar	got	0	-0.3	-0.3
2-chlorotoluene	C7H7Cl	4-chlorotoluene	C7H7Cl	0.798	429.41	2007	uno	kur	0	0.1	0.1
2-chlorotoluene	C7H7Cl	1,2-dimethylbenzene	C8H10	0.69	308.14	1987	dah	sin	0	12.6	12.5

toluene	C7H8	2-methylaniline	C7H9N	0.121	383.12	1985	gme		0	-2.8	-9.8
toluene	C7H8	2,6-dimethylpyridine	C7H9N	0.645	293.15	2006	ben	ait	0	0.5	0.5
toluene	C7H8	methylcyclohexane	C7H14	0.5	333.12	1961	sch		1	3.3	3.6
toluene	C7H8	methylcyclohexane	C7H14	0.778	379.66	1977	tym	kle	0	2.6	2.9
toluene	C7H8	heptane	C7H16	0.301	298.14	1965	kat	sun	0	-3.1	-2.7
toluene	C7H8	heptane	C7H16	0.773	303.14	1979	ash	cla	0	0.6	1
toluene	C7H8	heptane	C7H16	0.333	313.15	1994	gor		0	1.9	2.2
toluene	C7H8	octane	C8H18	0.764	363.82	1949	ber	pop	0	0.7	0.9
toluene	C7H8	octane	C8H18	0.699	344.59	1977	mih	kir	0	2	2.3
toluene	C7H8	2,2,4-trimethylpentane	C8H18	0.931	313.15	1993	gor	asm	0	-1.5	-1.3
2,6-dimethylpyridine	C7H9N	heptane	C7H16	0.71	353.15	2002	hak	ait	0	1	1.3
2,4-dimethylpyridine	C7H9N	1,2-dimethylbenzene	C8H10	0.45	373.12	1985	rog		1	-1.4	-1.4
2,6-dimethylpyridine	C7H9N	octane	C8H18	0.94	283.15	2005	ben	ait	0	-14	-13.8
3,5-dimethylpyridine	C7H9N	octane	C8H18	0.812	323.15	2005	ben	ait	0	-20	-19.4
benzylamine	C7H9N	water	H2O	0.102	323.15	2011	bel	mok	0	6.9	5.9
2,6-dimethylpyridine	C7H9N	water	H2O	0.776	298.14	1978	abe	nak	0	10.4	26.3
methylcyclohexane	C7H14	heptane	C7H16	0.286	323.15	1997	dah	wic	0	-0.2	-0.2
methylcyclohexane	C7H14	ethylbenzene	C8H10	0.676	353.13	1972	fun	cha	0	1	1.2
methylcyclohexane	C7H14	1,4-dimethylbenzene	C8H10	0.512	313.14	1980	asm	gor	0	2.7	2.9
heptane	C7H16	1,2-dimethylbenzene	C8H10	0.506	348.13	1980	dia	com	0	-0.2	0.1
heptane	C7H16	ethylbenzene	C8H10	0.784	313.09	1982	men	gre	0	0.3	0.4
heptane	C7H16	1,4-dimethylbenzene	C8H10	0.066	348.13	1980	dia	com	0	0.8	1.1
2,4-dimethylpentane	C7H16	octane	C8H18	0.684	293.15	1981	liu	dav	0	-2.2	-2.2
heptane	C7H16	octane	C8H18	0.641	328.15	1993	han	yan	0	-0.2	-0.2
benzene, ethenyl-	C8H8	1,2-dimethylbenzene	C8H10	0.256	357.56	2006	auc	lor	0	0.4	0.4
benzene, ethenyl-	C8H8	ethylbenzene	C8H10	0.829	356.67	2006	auc	lor	0	-0.1	0
benzene, ethenyl-	C8H8	1,4-dimethylbenzene	C8H10	0.693	329.88	2006	auc	lor	0	-0.5	-0.5
ethylbenzene	C8H10	1,4-dimethylbenzene	C8H10	0.633	409.8	1985	chi	mar	0	-0.8	-0.8
ethylbenzene	C8H10	1,3-dimethylbenzene	C8H10	0.218	332.45	1994	mon	llo	0	-1.5	-1.5
1,4-dimethylbenzene	C8H10	1,3-dimethylbenzene	C8H10	0.6	411.76	1971	kat	sat	0	0.3	0.3
ethylbenzene	C8H10	octane	C8H18	0.794	390.63	1955	yan	van	0	1.7	1.9

1,4-dimethylbenzene	C8H10	octane	C8H18	0.715	313.15	1994	gor		0	2.8	3.1
1-octene	C8H16	octane	C8H18	0.105	356.21	1980	kuu	too	0	0.2	0.2
hydrogen	H2	deuterium	H2	0.398	17.77	1974	ber	bog	0	-7.8	-7.8
water	H2O	hydrogen peroxide	H2O2	0.719	333.12	1952	sca	kav	0	4.3	4.1
water	H2O	hydrazine	H4N2	0.026	378.33	1952	bur		0	1.5	-0.4
nitrogen	N2	oxygen	O2	0.745	65.05	1955	arm	gol	0	-1.9	-1.8
oxygen	O2	ozone	O3	0.944	77.55	1955	jen	dip	0	3.1	2.7

^a Experimental data extracted from SOURCE Data Archival System; ^b Sorted according to Hill notation

Table S2. Deviations of excess enthalpies at temperature T , pressure P , and mole fraction of the first component x_1 calculated with Model I (Δ_I) and Model II (Δ_{II}) from the experimental values ^a

Component 1 ^b		Component 2 ^b		x_1	T / K	P / kPa	Reference code				$\Delta_I / \text{kJ}\cdot\text{mol}^{-1}$	$\Delta_{II} / \text{kJ}\cdot\text{mol}^{-1}$
Name	Formula	Name	Formula									
tetrachloromethane	CCl4	acetonitrile	C2H3N	0.214	298.15	101	2010	mar	por	0	0.12	0.10
tetrachloromethane	CCl4	ethanal	C2H4O	0.513	298.14	101	1985	mar		6	-0.03	-0.02
tetrachloromethane	CCl4	dimethyl sulfoxide	C2H6OS	0.650	298.14	101	1969	qui	pri	1	-0.06	-0.06
tetrachloromethane	CCl4	2-thiapropane	C2H6S	0.712	288.15	101	1975	gra	wil	0	0.49	0.50
tetrachloromethane	CCl4	1,4-dioxane	C4H8O2	0.700	298.14	101	1975	tan	dar	0	0.13	0.15
tetrachloromethane	CCl4	N-formylmorpholine	C5H9NO2	0.643	298.15	101	1990	gau	ste	0	0.08	0.09
tetrachloromethane	CCl4	cyclopentane	C5H10	0.326	308.14	101	1970	ewi	mar	4	-0.03	-0.03
tetrachloromethane	CCl4	2-pentanone	C5H10O	0.800	298.14	101	1977	kiy	ben	1	-0.07	-0.06
tetrachloromethane	CCl4	diethyl carbonate	C5H10O3	0.438	298.14	101	1987	gar	cob	0	0.08	0.09
tetrachloromethane	CCl4	benzene	C6H6	0.627	298.14	101	1966	mur	fuj	1	0.20	0.21
tetrachloromethane	CCl4	benzene	C6H6	0.500	298.14	101	1972	reh	bit	0	0.21	0.23
tetrachloromethane	CCl4	1-hexene	C6H12	0.559	298.14	101	1976	kar	gro	0	-0.15	-0.15
tetrachloromethane	CCl4	methylcyclopentane	C6H12	0.553	288.00	101	1981	fan	cen	0	-0.11	-0.11
tetrachloromethane	CCl4	1-heptyne	C7H12	0.400	298.14	101	1979	woy	rhe	0	0.12	0.13

tetrachloromethane	CCl4	octane	C8H18	0.205	293.15	101	1974	har	tho	0	-0.17	-0.17
tribromomethane	CHBr3	tetrahydrofuran	C4H8O	0.263	298.14	101	1987	bec	hal	0	0.26	0.23
trichloromethane	CHCl3	ethanol	C2H6O	0.485	303.14	101	1975	sha	abb	0	-0.60	-0.66
trichloromethane	CHCl3	acetone	C3H6O	0.136	298.14	101	1981	nag	tam	0	-0.11	-0.12
trichloromethane	CHCl3	tetrahydrofuran	C4H8O	0.375	298.14	101	1971	bec	kie	0	0.36	0.31
trichloromethane	CHCl3	tetrahydrothiophene	C4H8S	0.502	298.14	101	1977	wag	mal	0	0.40	0.36
trichloromethane	CHCl3	benzene	C6H6	0.337	297.99	101	1971	ras	nat	0	0.14	0.14
trichloromethane	CHCl3	1-formylpiperidine	C6H11NO	0.992	298.15	101	1990	gau	ste	0	-0.08	-0.08
trichloromethane	CHCl3	heptane	C7H16	0.208	303.11	101	1975	sha	abb	0	-0.23	-0.23
trichloromethane	CHCl3	1,2-dimethylbenzene	C8H10	0.457	298.14	101	1973	abe		0	0.59	0.58
dibromomethane	CH2Br2	benzene	C6H6	0.951	308.14	101	1984	sin	nig	1	-0.03	-0.04
dichloromethane	CH2Cl2	acetone	C3H6O	0.072	303.13	101	1966	win	van	0	-0.13	-0.14
dichloromethane	CH2Cl2	methyl ethanoate	C3H6O2	0.362	303.13	101	1966	win	van	0	-0.56	-0.59
dichloromethane	CH2Cl2	1,4-dioxane	C4H8O2	0.997	303.14	101	1974	van	abb	0	-0.01	-0.01
methanoic acid	CH2O2	benzene	C6H6	0.995	300.04	101	1973	lak	kap	0	-0.01	-0.02
iodomethane	CH3I	hexane	C6H14	0.358	303.14	101	1987	mun	oti	0	-0.30	-0.28
formamide	CH3NO	1-hexanol	C6H14O	0.191	298.15	101	2003	zar	ilo	0	-0.62	-1.54
nitromethane	CH3NO2	1-butanol	C4H10O	0.297	298.15	101	1990	bat	row	0	-0.74	-0.84
nitromethane	CH3NO2	1,4-dimethylbenzene	C8H10	0.296	298.14	101	1985	mar		9	-2.85	-2.92
methanol	CH4O	acetone	C3H6O	0.400	298.15	101	1994	nag		4	-0.56	-0.38
methanol	CH4O	dimethylformamide	C3H7NO	0.718	298.14	101	1989	cha	dai	2	-0.14	0.15
methanol	CH4O	tetrahydrofuran	C4H8O	0.072	298.14	101	1966	arm	ban	0	-0.26	-0.17
methanol	CH4O	N-methyl-2-pyrrolidone	C5H9NO	0.172	298.15	101	1999	lop	gar	0	0.17	0.38
methanol	CH4O	1,3-dichlorobenzene	C6H4Cl2	0.174	298.15	101	1993	let	nev	0	-0.39	-0.49
methanol	CH4O	benzene	C6H6	0.952	298.14	101	1969	coc		0	-0.05	-0.06
methanol	CH4O	benzene	C6H6	0.676	298.14	101	1969	ves	pic	0	-0.28	-0.35
methanol	CH4O	cyclohexane	C6H12	0.920	298.15	101	1998	fri	sch	0	-0.15	-0.17
methanol	CH4O	cyclohexane	C6H12	0.659	323.14	101	1985	dai	cha	1	-0.54	-0.61
methanol	CH4O	2,6-dimethylpyridine	C7H9N	0.818	298.14	101	1985	tou	nak	0	0.97	1.11
methanol	CH4O	ethylbenzene	C8H10	0.326	308.13	101	1961	mra	van	0	-0.47	-0.59

methanol	CH4O	water	H2O	0.597	293.14	101	1962	kat		1	0.35	0.21
tetrachloroethene	C2Cl4	2-methoxyethanol	C3H8O2	0.965	298.15	101	1994	ven	pra	0	-0.26	-0.28
tetrachloroethene	C2Cl4	1,3-dimethylbenzene	C8H10	0.550	298.14	101	1980	han	ben	1	0.05	0.05
trichloroethene	C2HCl3	1-hexanol	C6H14O	0.456	298.15	101	1997	ilo		0	0.09	0.04
1,1,2,2-tetrachloroethane	C2H2Cl4	ethyl butanoate	C6H12O2	0.177	298.15	101	1991	ort		2	-0.35	-0.37
1,1,1-trichloroethane	C2H3Cl3	dimethylformamide	C3H7NO	0.355	298.15	101	2000	ven	ram	0	-0.56	-0.56
1,1,1-trichloroethane	C2H3Cl3	1,4-dioxane	C4H8O2	0.609	298.15	101	1992	sur	kri	0	-0.64	-0.64
1,1,1-trichloroethane	C2H3Cl3	cyclohexane	C6H12	0.463	298.14	101	1984	chr	gme	1	-0.04	-0.03
2,2,2-trifluoroethanol	C2H3F3O	tetrahydropyran	C5H10O	0.935	283.15	101	2003	per	mai	0	-0.05	0.03
acetonitrile	C2H3N	1-butanol	C4H10O	0.894	298.14	101	1966	mur	fuj	0	-0.46	-0.38
acetonitrile	C2H3N	hexane	C6H14	0.005	298.14	101	1981	lak	man	1	-0.03	-0.02
acetonitrile	C2H3N	toluene	C7H8	0.702	321.34	101	1984	chr	gme	1	-0.03	-0.06
acetonitrile	C2H3N	1-heptanol	C7H16O	0.299	298.15	101	2008	che	dag	0	-0.73	-0.63
1,2-dibromoethane	C2H4Br2	cyclohexane	C6H12	0.421	298.14	101	1976	mah	kon	0	0.03	0.03
1,2-dichloroethane	C2H4Cl2	cyclohexane	C6H12	0.058	308.14	101	1983	ban	val	0	0.03	0.04
1,2-dichloroethane	C2H4Cl2	2-heptanone	C7H14O	0.396	298.15	101	1990	kec	dub	0	0.12	0.10
1,2-dichloroethane	C2H4Cl2	heptane	C7H16	0.391	303.15	101	1990	cha	kat	0	-0.10	-0.09
ethanoic acid	C2H4O2	1,3-dioxacyclopentane	C3H6O2	0.169	298.14	101	1989	com	fra	0	-0.52	-0.47
ethanoic acid	C2H4O2	pyridine	C5H5N	0.959	298.14	101	1972	abr	mir	0	0.91	0.92
nitroethane	C2H5NO2	benzene	C6H6	0.312	298.14	101	1978	cle	hsu	0	0.08	0.02
nitroethane	C2H5NO2	cyclohexane	C6H12	0.238	297.15	101	1989	mar	rog	0	0.12	0.10
ethanol	C2H6O	dimethyl sulfoxide	C2H6OS	0.151	298.14	101	1989	cha	dai	2	-0.59	-0.38
ethanol	C2H6O	1,2-ethanediol	C2H6O2	0.350	308.15	101	1999	kra	ulb	1	-0.32	-0.32
ethanol	C2H6O	dimethylformamide	C3H7NO	0.737	298.14	101	1989	cha	dai	2	-0.68	-0.42
ethanol	C2H6O	butanone	C4H8O	0.613	308.14	101	1976	nag	oht	1	-0.97	-0.81
ethanol	C2H6O	1,2-butanediol	C4H10O2	0.450	323.15	101	1999	kra	ulb	1	-0.25	-0.25
ethanol	C2H6O	2,4-pentanedione	C5H8O2	0.452	298.15	100	2008	li	yan	0	-0.91	-0.76
ethanol	C2H6O	tetrahydropyran	C5H10O	0.373	298.15	101	1995	let	gov	1	-1.07	-0.85
ethanol	C2H6O	1-pentanol	C5H12O	0.959	298.14	101	1968	ram	rue	0	-0.01	-0.01
ethanol	C2H6O	1,3-dichlorobenzene	C6H4Cl2	0.341	298.15	101	1993	let	nev	0	-0.61	-0.71

ethanol	C2H6O	cyclohexane	C6H12	0.499	293.14	101	1966	kle		1	-0.04	-0.10
ethanol	C2H6O	2,2-dimethylbutane	C6H14	0.111	298.14	101	1985	per	gra	0	-0.08	-0.14
ethanol	C2H6O	1,4-dimethylbenzene	C8H10	0.970	318.14	0	1980	sto	fre	0	-0.05	-0.06
ethanol	C2H6O	water	H2O	0.104	293.15	101	1970	kha	byv	0	0.69	0.62
dimethyl sulfoxide	C2H6OS	dimethylformamide	C3H7NO	0.025	298.15	101	1993	nak	chu	1	-0.02	-0.02
dimethyl sulfoxide	C2H6OS	1,4-dimethylbenzene	C8H10	0.827	312.99	101	1983	nis	kai	0	-0.75	-0.77
dimethyl sulfoxide	C2H6OS	1-octyne	C8H14	0.303	298.15	101	1999	let	whi	0	-0.71	-0.75
dimethyl sulfoxide	C2H6OS	water	H2O	0.250	298.15	101	1997	miy	nak	0	0.16	0.66
1,2-ethanediol	C2H6O2	N-methylacetamide	C3H7NO	0.580	413.15	101	1997	deh	fis	0	-0.02	-0.80
1,2-ethanediol	C2H6O2	1-butanol	C4H10O	0.677	298.14	101	1979	jim	paz	0	-0.56	-0.57
1,2-ethanediol	C2H6O2	water	H2O	0.550	285.65	101	1999	kra	ulb	0	0.24	0.09
2,3-dithiabutane	C2H6S2	cyclohexane	C6H12	0.379	298.15	101	1994	mar	mar	0	-0.08	-0.07
N,N-dimethylhydrazine	C2H8N2	water	H2O	0.615	278.15	101	1993	fer	laa	0	3.28	2.33
1-propanol, 2,2,3,3-tetrafluoro-1-chloro-2,3-epoxypropane	C3H4F4O	benzene	C6H6	0.424	298.14	101	1966	bra	oni	0	-1.60	-1.67
propanenitrile	C3H5ClO	heptane	C7H16	0.911	298.14	101	1986	kra	koc	0	-0.17	-0.17
propanenitrile	C3H5N	benzene	C6H6	0.136	298.15	101	2010	mar	por	0	-0.04	-0.05
propanenitrile	C3H5N	ethyl 1,1-dimethylethyl ether	C6H14O	0.801	298.44	101	2013	laa	pok	0	-0.03	-0.04
1,2-dibromopropane	C3H6Br2	benzene	C6H6	0.723	298.14	101	1987	rui	roy	0	-0.13	-0.13
1,3-dibromopropane	C3H6Br2	heptane	C7H16	0.681	298.15	101	1993	ort	pla	2	-0.22	-0.21
1,3-dichloropropane	C3H6Cl2	ethyl methanoate	C3H6O2	0.846	298.15	101	2002	ort		0	-0.11	-0.11
1,3-dichloropropane	C3H6Cl2	butyl methanoate	C5H10O2	0.313	298.15	101	2007	ort	mar	0	0.30	0.30
1,3-dichloropropane	C3H6Cl2	diethyl carbonate	C5H10O3	0.939	298.15	101	1995	com	fra	1	-0.02	-0.02
acetone	C3H6O	1-propanol	C3H8O	0.799	303.15	101	1990	ton	zha	0	-0.81	-0.66
acetone	C3H6O	cyclohexane	C6H12	0.520	298.14	101	1975	han	fen	2	-0.72	-0.73
acetone	C3H6O	2-heptanone	C7H14O	0.546	303.14	101	1971	ram	til	0	-0.18	-0.18
acetone	C3H6O	water	H2O	0.472	318.14	101	1989	fre		0	-0.67	-0.45
1,3-dioxacyclopentane	C3H6O2	butanone	C4H8O	0.720	288.15	101	1989	com		0	-0.10	-0.10
methyl ethanoate	C3H6O2	1-chlorobutane	C4H9Cl	0.290	298.15	101	1990	ave	rou	0	-0.45	-0.46

1,3-dioxacyclopentane	C3H6O2	1-butanol	C4H10O	0.850	298.15	101	1999	bro	cal	1	-1.10	-0.97
methyl ethanoate	C3H6O2	2-methyl-2-propanol	C4H10O	0.541	318.15	101	2004	ort	esp	2	-1.71	-1.58
ethyl methanoate	C3H6O2	benzene	C6H6	0.950	298.15	101	1997	hu	tam	1	-0.08	-0.08
ethyl methanoate	C3H6O2	benzene	C6H6	0.650	298.15	101	1997	hu	tam	1	-0.38	-0.37
propanoic acid	C3H6O2	cyclohexane	C6H12	0.921	313.15	101	1996	com	fra	0	0.11	0.10
1,3-dioxacyclopentane	C3H6O2	2,2,4-trimethylpentane	C8H18	0.090	298.15	101	1993	fra	com	1	-0.07	-0.07
1-chloropropane	C3H7Cl	benzene	C6H6	0.925	298.14	101	1989	gar	gar	1	0.00	0.00
dimethylformamide	C3H7NO	2-methyl-1-propanol	C4H10O	0.577	298.15	101	1991	cha	wan	0	-1.12	-0.80
dimethylformamide	C3H7NO	1,3-cyclopentadiene	C5H6	0.684	298.14	101	1983	ked	sem	0	-0.46	-0.45
dimethylformamide	C3H7NO	water	H2O	0.301	318.15	101	1995	zai	kre	0	0.66	0.96
1-nitropropane	C3H7NO2	chlorobenzene	C6H5Cl	0.702	298.14	101	1978	nic	eck	0	-0.10	-0.14
2-nitropropane	C3H7NO2	cyclohexane	C6H12	0.078	298.14	101	1984	mar	all	0	-0.14	-0.15
2-propanol	C3H8O	1-propanol	C3H8O	0.033	298.14	101	1970	pol	mur	1	0.01	0.01
2-propanol	C3H8O	1,2-propanediamine	C3H10N2	0.204	298.15	101	2006	kim	kit	0	1.15	0.49
1-propanol	C3H8O	1,3-propanediamine	C3H10N2	0.337	298.15	101	2006	kim	kit	0	1.97	0.97
1-propanol	C3H8O	1,2-propanediamine	C3H10N2	0.985	298.15	101	2006	kim	kit	0	0.22	0.17
2-propanol	C3H8O	ethyloxirane	C4H8O	0.532	298.15	101	1996	com	fra	2	-1.41	-1.29
1-propanol	C3H8O	1,4-dioxane	C4H8O2	0.250	298.15	101	1999	cal	bro	0	-1.43	-1.22
1-propanol	C3H8O	N-methyl-2-pyrrolidone	C5H9NO	0.347	298.15	101	2001	let	lac	0	-0.64	-0.32
2-propanol	C3H8O	3-pentanone	C5H10O	0.843	298.15	101	1995	let	nev	1	-0.81	-0.74
1-propanol	C3H8O	propyl ethanoate	C5H10O2	0.800	308.14	101	1975	bel	bal	0	-0.95	-0.85
1-propanol	C3H8O	1,1-dimethylethyl methyl ether	C5H12O	0.400	298.15	101	1994	zhu	she	4	-0.84	-0.60
2-propanol	C3H8O	1,3-dichlorobenzene	C6H4Cl2	0.330	298.15	101	1993	let	nev	0	-1.01	-1.09
1-propanol	C3H8O	1,3-dichlorobenzene	C6H4Cl2	0.226	298.15	101	1993	let	nev	0	-0.69	-0.77
2-propanol	C3H8O	cyclohexane	C6H12	0.072	298.15	101	1996	sin	kal	3	-0.04	-0.08
1-propanol	C3H8O	1-hexanol	C6H14O	0.554	298.15	101	1993	lop	leg	0	-0.03	-0.03
1-propanol	C3H8O	heptane	C7H16	0.901	323.15	101	2003	lie	lin	0	-0.21	-0.24
2-propanol	C3H8O	1,4-dimethylbenzene	C8H10	0.800	298.15	101	1996	sin	kal	0	-0.40	-0.44
1-propanol	C3H8O	1-octene	C8H16	0.520	298.15	101	1993	let	mer	1	-0.23	-0.31

1-methylsulfinyl-2-thiapropane	C3H8OS2	1-pentanamine	C5H13N	0.133	298.15	101	2003	kim	mat	0	-0.10	0.03
1-methylsulfinyl-2-thiapropane	C3H8OS2	ethylbenzene	C8H10	0.032	298.15	101	1999	kim	suz	0	-0.05	-0.05
1-methylsulfinyl-2-thiapropane	C3H8OS2	ethylbenzene	C8H10	0.180	298.15	101	1999	kim	suz	0	-0.22	-0.23
1,3-propanediol	C3H8O2	2-propanamine 1,2-propanediyl	C3H9N	0.141	298.15	101	2006	kim	kit	0	2.82	2.11
2-methoxyethanol	C3H8O2	carbonate	C4H6O3	0.763	313.15	101	2000	com	fra	0	-0.34	-0.34
2-methoxyethanol	C3H8O2	diethyl carbonate	C5H10O3	0.060	313.15	101	1999	fra	cas	0	-0.32	-0.29
1,2-propanediol	C3H8O2	1-heptanol	C7H16O	0.853	298.14	101	1974	gar	paz	0	-0.26	-0.27
1,2-propanediol	C3H8O2	water	H2O	0.281	298.14	101	1977	mat	tou	0	0.52	0.35
3-amino-1-propanol	C3H9NO	water	H2O	0.030	323.15	101	2007	mun	hen	1	0.65	0.60
1,3-propanediamine	C3H10N2	toluene	C7H8	0.705	303.15	101	2001	kec	dah	0	-0.84	-0.84
.gamma.-butyrolactone	C4H6O2	1-hexanol	C6H14O	0.470	298.15	101	1990	ram	ram	0	-1.48	-1.34
2,3-butanedione	C4H6O2	water	H2O	0.006	313.15	101	2012	doh	reh	0	0.07	0.07
(R)-4-methyl-1,3-dioxolan-2-one	C4H6O3	(S)-4-methyl-1,3-dioxolan-2-one	C4H6O3	0.537	298.15	101	2006	kim	kha	0	0.01	0.01
1,2-propanediyl carbonate	C4H6O3	1,2-dimethylbenzene	C8H10	0.600	288.15	101	1975	shc	ten	1	-0.27	-0.30
butanenitrile	C4H7N	cyclohexane	C6H12	0.887	303.14	101	1983	val	gra	0	-0.17	-0.18
butanenitrile	C4H7N	methylcyclohexane	C7H14	0.520	298.14	101	1980	ale	ale	0	-0.32	-0.33
2-pyrrolidinone	C4H7NO	1-pentanol	C5H12O	0.101	303.15	101	1997	meh	cha	0	-0.62	-0.79
tetrahydrofuran	C4H8O	benzene	C6H6	0.600	298.15	101	2006	gin	mar	0	-0.01	-0.01
butanone	C4H8O	heptane	C7H16	0.769	328.19	101	1984	fuc	kre	0	-0.46	-0.47
tetrahydrofuran	C4H8O	water-d2	H2O	0.230	283.17	101	1973	gle	wat	0	-0.14	-0.02
tetrahydrofuran	C4H8O	water	H2O	0.805	297.99	101	1971	nak	shi	0	-1.09	-0.83
propyl methanoate	C4H8O2	1,5-dichloropentane	C5H10Cl2	0.953	298.15	101	2009	mar	ort	0	0.00	0.00
1,3-dioxane	C4H8O2	benzene	C6H6	0.064	298.15	101	1997	tak	oga	0	-0.06	-0.06
1,4-dioxane	C4H8O2	aniline	C6H7N	0.982	293.15	101	1984	chr	gme	1	-0.10	-0.04
1,4-dioxane	C4H8O2	cyclohexanone	C6H10O	0.800	298.15	101	2000	tam	osa	1	-0.20	-0.20
methyl propanoate	C4H8O2	cyclohexane	C6H12	0.529	298.15	101	1998	mar	por	0	-0.52	-0.53
ethyl ethanoate	C4H8O2	1-bromohexane	C6H13Br	0.632	303.14	101	1980	oti	tom	0	-0.33	-0.34

2-methyl-1,3-dioxolane	C4H8O2	heptane	C7H16	0.239	298.14	101	1979	mey	giu	0	-0.41	-0.41
1,4-dioxane	C4H8O2	2,2,4-trimethylpentane	C8H18	0.090	298.15	101	1997	tak	oga	0	-0.21	-0.21
2-bromo-2-methylpropane	C4H9Br	cyclohexane	C6H12	0.572	283.15	101	1980	pei	gra	0	0.07	0.07
1-chlorobutane	C4H9Cl	benzene	C6H6	0.078	298.15	101	1991	sin	kal	0	-0.03	-0.03
2-chlorobutane	C4H9Cl	hexane	C6H14	0.250	308.14	101	1978	lai	doa	0	-0.08	-0.08
1-chlorobutane	C4H9Cl	1-heptanol	C7H16O	0.656	298.15	101	1999	san	bal	0	-0.62	-0.68
N,N-dimethylacetamide	C4H9NO	1-chlorohexane	C6H13Cl	0.304	308.15	101	2007	gar	emb	0	-0.55	-0.57
1-butanol	C4H10O	2-methyl-2-propanol	C4H10O	0.159	299.14	101	1973	mur	ben	0	0.28	0.28
(RS)-2-butanol	C4H10O	2-(N,N-dimethylamino)ethanol	C4H11NO	0.769	298.15	101	1995	yan	zha	0	0.36	0.31
(RS)-2-butanol	C4H10O	pyrrolidone	C5H9NO	0.603	298.15	101	2001	let	lac	0	-1.07	-0.73
2-methyl-2-propanol	C4H10O	butyl methanoate	C5H10O2	0.837	299.15	101	2005	ort	esp	0	-1.00	-0.96
1-butanol	C4H10O	diethyl carbonate	C5H10O3	0.181	308.15	101	1999	com	fra	1	-1.16	-1.05
diethyl ether	C4H10O	1,1-dimethylethyl methyl ether	C5H12O	0.750	298.15	101	1997	lia	zha	0	-0.02	-0.02
diethyl ether	C4H10O	3-methyl-1-butanol	C5H12O	0.571	298.27	101	1925	hir		0	-1.10	-0.88
(RS)-2-butanol	C4H10O	chlorobenzene	C6H5Cl	0.165	298.14	101	1989	cha	dai	0	-0.80	-0.86
1-butanol	C4H10O	cyclohexane	C6H12	0.774	288.15	101	1983	fre		0	-0.03	-0.06
1-butanol	C4H10O	cyclohexane	C6H12	0.057	308.14	101	1970	bel	kur	0	-0.18	-0.22
2-methyl-2-propanol	C4H10O	cyclohexane	C6H12	0.003	318.14	101	1983	fre		0	-0.03	-0.03
2-methyl-2-propanol	C4H10O	cyclohexane	C6H12	0.061	318.14	101	1983	fre		0	-0.36	-0.40
1-butanol	C4H10O	2-methylpentane	C6H14	0.501	298.15	101	1994	gar	san	0	-0.08	-0.14
2-methyl-1-propanol	C4H10O	diethyl 1,3-propanedioate	C7H12O4	0.200	288.15	101	2010	wan	gao	2	-1.71	-1.58
2-methyl-1-propanol	C4H10O	heptane	C7H16	0.150	298.14	100	1986	osw	sch	0	-0.22	-0.28
1-butanol	C4H10O	ethylbenzene	C8H10	0.227	298.14	101	1961	mra	van	0	-0.60	-0.68
1-butanol	C4H10O	water	H2O	0.140	298.00	100	1991	ben	hei	0	0.02	-0.08
2-ethoxyethanol	C4H10O2	cyclohexane	C6H12	0.624	308.15	101	2006	mis	tsi	0	-0.69	-0.72
diethylamine	C4H11N	benzene	C6H6	0.545	293.15	101	1969	sie	gro	0	0.02	-0.05
pyridine	C5H5N	N-	C5H13NO2	0.485	298.15	101	2013	pou	sha	0	-0.21	-0.08

		methyldiethanolamine										
pyridine	C5H5N	chlorobenzene	C6H5Cl	0.100	313.14	101	1979	mal	pat	0	-0.05	-0.05
pyridine	C5H5N	hexane	C6H14	0.316	298.15	101	1992	kec	dub	0	-0.53	-0.53
pyridine	C5H5N	2,2,4-trimethylpentane	C8H18	0.799	298.14	101	1972	kon		0	-0.49	-0.49
pyridine	C5H5N	water	H2O	0.015	298.14	101	1973	sha	abd	0	0.06	0.06
2-methyl-1,3-butadiene	C5H8	pentane	C5H12	0.300	293.15	101	1977	gue	bit	0	0.25	0.25
2,4-pentanedione	C5H8O2	1-pentanol	C5H12O	0.050	298.15	100	2008	li	yan	1	-0.17	-0.13
.gamma.-valerolactone	C5H8O2	toluene	C7H8	0.912	293.15	101	2002	bjo	sid	1	-0.09	-0.10
1-oxacyclohexan-2-one	C5H8O2	toluene	C7H8	0.855	293.15	101	2002	bjo	sid	1	-0.20	-0.20
cyclopentane	C5H10	2,3-dimethylbutane	C6H14	0.071	288.15	101	1973	ewi	mar	1	0.00	0.00
cyclopentane	C5H10	octane	C8H18	0.443	298.19	101	1983	let	hey	0	-0.08	-0.08
cyclopentanol	C5H10O	cyclohexane	C6H12	0.345	298.14	101	1974	ben	ana	0	-0.21	-0.27
2-pentanone	C5H10O	1-chlorohexane	C6H13Cl	0.450	298.15	101	1991	pic	men	0	-0.21	-0.21
tetrahydropyran	C5H10O	hexane	C6H14	0.497	308.15	101	2010	siw	dim	1	-0.35	-0.35
pentanal	C5H10O	hexane	C6H14	0.304	298.14	101	1983	ing	fer	0	-0.38	-0.38
tetrahydropyran	C5H10O	1-hexanol	C6H14O	0.448	298.15	101	1994	alo	cal	0	-1.36	-1.12
3-pentanone	C5H10O	triethylamine	C6H15N	0.224	303.14	101	1986	kok		1	-0.29	-0.29
propyl ethanoate	C5H10O2	hexane	C6H14	0.134	298.14	101	1974	gro	bal	0	-0.16	-0.16
ethyl propanoate	C5H10O2	N-propyl-1-propanamine	C6H15N	0.511	298.14	101	1989	nun	bar	0	0.04	-0.03
diethyl carbonate	C5H10O3	ethoxybenzene	C8H10O	0.610	313.15	101	2000	fra	com	0	-0.30	-0.30
1-fluoropentane	C5H11F	hexane	C6H14	0.778	298.15	101	1991	art	fer	13	-0.14	-0.14
N,N-diethylformamide	C5H11NO	toluene	C7H8	0.825	298.14	101	1974	uki	tan	0	-0.01	-0.01
1-nitropentane	C5H11NO2	benzene	C6H6	0.341	298.14	101	1978	hsu	cle	0	0.17	0.14
pentane	C5H12	1,6-dibromohexane	C6H12Br2	0.408	298.15	101	1993	ort	pla	2	-0.36	-0.35
1-pentanol	C5H12O	1-pentanamine	C5H13N	0.727	15.00	101	1979	sim	ver	0	1.86	1.27
1-pentanol	C5H12O	aniline	C6H7N	0.718	298.15	101	1990	wan	cha	2	-1.28	-1.69
1,1-dimethylethyl methyl ether	C5H12O	1-hexene	C6H12	0.202	308.15	101	1997	let	dom	0	-0.11	-0.11
1-pentanol	C5H12O	1,6-dichlorohexane	C6H12Cl2	0.553	298.15	101	1998	med	fer	0	-0.91	-0.99

1-pentanol	C5H12O	1,3-dimethylbenzene	C8H10	0.401	298.14	101	1985	rod	paz	0	-0.54	-0.62
1,1-dimethylethyl methyl ether	C5H12O	1-octyne	C8H14	0.644	298.15	101	1999	let	gov	0	-0.07	-0.07
diethoxymethane	C5H12O2	octane	C8H18	0.796	298.14	101	1979	mey	giu	1	-0.14	-0.15
1,2-dichlorobenzene	C6H4Cl2	chlorobenzene	C6H5Cl	0.600	298.14	101	1979	tan	ben	0	-0.05	-0.05
1,2-dichlorobenzene	C6H4Cl2	1,2-dimethylbenzene	C8H10	0.402	308.14	101	1979	mah	khu	0	0.00	0.00
bromobenzene	C6H5Br	cyclohexane	C6H12	0.550	298.14	101	1979	mur	kim	0	-0.10	-0.09
chlorobenzene	C6H5Cl	benzonitrile	C7H5N	0.676	298.14	101	1974	tan	mur	0	-0.01	-0.01
fluorobenzene	C6H5F	methylcyclohexane	C7H14	0.800	283.10	101	1968	bha	muk	0	-0.02	-0.01
benzene	C6H6	cyclohexane	C6H12	0.802	298.14	101	1976	ell	wor	0	-0.05	-0.04
benzene	C6H6	cyclohexane	C6H12	0.656	328.13	101	1966	sab	bel	0	0.00	0.01
benzene	C6H6	2-methylpentane	C6H14	0.726	298.14	101	1973	paz		0	-0.19	-0.17
benzene	C6H6	1-fluoro-2-methylbenzene	C7H7F	0.400	303.14	101	1985	oti	tol	1	-0.08	-0.08
benzene	C6H6	heptane	C7H16	0.691	297.99	101	1971	let	bay	0	-0.14	-0.13
benzene	C6H6	1,3-dimethylbenzene	C8H10	0.780	323.14	101	1972	paz	her	0	-0.13	-0.13
4-methylpyridine	C6H7N	hexane	C6H14	0.317	298.15	101	1992	kec	dub	0	-0.44	-0.44
2-methylpyridine	C6H7N	ethylcyclohexane	C8H16	0.600	298.14	101	1972	woy		0	-0.35	-0.35
3-methylpyridine	C6H7N	octane	C8H18	0.722	298.15	101	1992	kas	wil	0	-0.49	-0.49
3-methylpyridine	C6H7N	water	H2O	0.294	298.15	101	1998	mar	gie	0	0.80	0.91
cyclohexene	C6H10	cyclohexane	C6H12	0.457	298.14	101	1982	gro	ing	0	0.00	0.00
1-hexyne	C6H10	1-methyl-1-(1-methylethoxy)ethane	C6H14O	0.486	298.15	101	1999	let	gov	0	-0.09	-0.10
2,5-hexanedione	C6H10O2	heptane	C7H16	0.953	298.14	101	1989	mar	der	0	-0.37	-0.38
(E)-2-hexene	C6H12	(E)-3-hexene	C6H12	0.237	298.14	101	1975	woy		0	0.00	0.00
1-hexene	C6H12	3-methylpentane	C6H14	0.200	298.15	101	2004	wan	ben	0	0.03	0.03
1-hexene	C6H12	2-methylpentane	C6H14	0.200	298.15	101	2004	wan	ben	0	0.02	0.02
cyclohexane	C6H12	hexane	C6H14	0.034	298.14	101	1970	ewi	mar	1	-0.02	-0.02
cyclohexane	C6H12	hexane	C6H14	0.200	298.14	101	1987	bao	you	0	-0.12	-0.12
cyclohexane	C6H12	hexane	C6H14	0.357	298.14	79	1988	elk	whi	0	-0.18	-0.18
cyclohexane	C6H12	hexane	C6H14	0.500	298.14	101	1970	ewi	mar	1	-0.21	-0.21
cyclohexane	C6H12	1-hexanol	C6H14O	0.528	298.14	101	1987	ves	doh	0	-0.26	-0.31

cyclohexane	C6H12	toluene	C7H8	0.830	298.14	101	1970	paz	bal	0	0.13	0.14
cyclohexane	C6H12	toluene	C7H8	0.256	298.14	101	1965	wat	mcl	0	-0.03	-0.03
cyclohexane	C6H12	1,4-dimethylbenzene	C8H10	0.905	298.14	101	1982	nag	oga	0	-0.06	-0.05
cyclohexane	C6H12	1-octyne	C8H14	0.924	298.14	101	1988	let	tay	0	-0.05	-0.05
cyclohexanol	C6H12O	water	H2O	0.002	298.15	101	2002	hov	rou	0	0.03	0.03
propyl propanoate	C6H12O2	hexane	C6H14	0.589	298.14	101	1989	lor	leg	0	-0.29	-0.29
butyl ethanoate	C6H12O2	ethylbenzene	C8H10	0.200	298.15	101	2009	ort	nav	0	-0.05	-0.05
butyl ethanoate	C6H12O2	1-octyne	C8H14	0.471	298.15	101	1992	kir	kuu	0	-0.19	-0.20
2,2-dimethylbutane	C6H14	2-ethyl-1-butanol	C6H14O	0.400	298.14	101	1982	kim	ben	0	-0.25	-0.30
2,3-dimethylbutane	C6H14	2-methyl-1-pentanol	C6H14O	0.350	298.14	101	1982	kim	ben	1	-0.17	-0.21
dipropyl ether	C6H14O	heptane	C7H16	0.100	298.14	101	1983	kim	dar	0	-0.03	-0.03
2-butoxyethanol	C6H14O2	water	H2O	0.613	322.13	101	1994	lim	whi	0	-0.38	-0.59
N-propyl-1-propanamine	C6H15N	heptane	C7H16	0.529	298.14	101	1984	paz	sar	0	-0.17	-0.16
triethylamine	C6H15N	water	H2O	0.495	288.15	101	1968	ber	lar	0	1.66	1.73
benzaldehyde	C7H6O	heptane	C7H16	0.281	298.14	101	1982	fer	mar	0	-0.12	-0.11
toluene	C7H8	2,6-dimethylpyridine	C7H9N	0.552	303.15	101	2006	ben	ait	0	-0.06	-0.06
toluene	C7H8	1,2-dimethylbenzene	C8H10	0.370	298.14	101	1969	mur	lam	0	-0.03	-0.03
diethyl 1,3-propanedioate	C7H12O4	heptane	C7H16	0.799	288.15	101	2010	wan	gao	2	-0.50	-0.52
cycloheptane	C7H14	heptane	C7H16	0.907	298.15	101	1992	por		1	-0.11	-0.11
heptane	C7H16	1-heptanol	C7H16O	0.513	298.14	101	1989	ami	leg	0	-0.12	-0.18
1,4-dimethylbenzene	C8H10	1,3-dimethylbenzene	C8H10	0.310	298.14	101	1970	lam	mur	0	0.01	0.01

^a Experimental data extracted from SOURCE Data Archival System; ^b Sorted according to Hill notation

Table S3. Deviations of activity coefficients at temperature T , pressure P , and mole fraction of the first component x_1 calculated with Model I (γ_I) and Model II (γ_{II}) from the experimental values ^a

Component 1 ^b		Component 2 ^b		x_1	T / K	P / kPa	Reference code			$\ln \gamma_1 - \ln \gamma_{\text{exp}}$	$\ln \gamma_{\text{II}} - \ln \gamma_{\text{exp}}$	
Name	Formula	Name	Formula									
tetrachloromethane	CCl4	2-methyl-1,3-butadiene	C5H8	0	293.15	0	1982	tho	new	1	0.12	0.13
methanol	CH4O	octane	C8H18	0.014	293.15	0	1992	wob	hra	0	-0.81	-0.77
ethanoic acid	C2H4O2	N-methyl-2-pyrrolidone	C5H9NO	0.597	390.85	0	2011	pin	pen	0	0.28	0.29
ethanol	C2H6O	ethyl ethanoate	C4H8O2	0	312.99	0	1982	tho	new	0	-0.66	-0.14
propene	C3H6	1-propanol	C3H8O	1	300.03	0	2004	miy		0	-0.68	-0.68
propane	C3H8	3-methylphenol	C7H8O	0	309.99	0	2010	miy	ash	0	-0.9	-0.9
2-propanol	C3H8O	toluene	C7H8	0	313.14	0	1989	kno	tie	0	-0.04	0.51
2-butanone oxime	C4H9NO	heptane	C7H16	0.045	368.13	101	1968	gei	koe	0	-0.02	-0.04
(RS)-2-butanol	C4H10O	water	H2O	0.017	293.15	0	1986	sag	lau	0	0.84	0.58
2-furaldehyde	C5H4O2	heptane	C7H16	0	298.15	0	2012	fur	coe	0	-0.95	-0.94
benzene	C6H6	octane	C8H18	0.47	338.13	40	1968	els	lu	0	0.05	0.05
triethylamine	C6H15N	octane	C8H18	1	298.15	0	2000	cas	eik	0	0.04	0.04

^a Experimental data extracted from SOURCE Data Archival System; ^b Sorted according to Hill notation

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