Benzenemethanol, «alpha»-methyl-

Other names:	(1-Hydroxyethyl)benzene
	.alpha.-methylbenzyl alcohol
	.alpha.-phenylethyl alcohol
	1-Fenylethanol
	1-Phenethyl alcohol
	1-Phenyl-1-hydroxyethane
	1-Phenylethanol
	1-Phenylethyl alcohol
	Benzyl alcohol, «alpha»-methyl-
	Benzyl alcohol, Â«alphaÂ»-methyl-
	Ethanol, 1-phenyl-
	Fenyl-methylkarbinol
	Methanol, methylphenyl-
	Methylphenylcarbinol
	NCI-C55685
	NSC 25502
	Phenylmethylcarbinol
	Styrallyl alcohol
	Styralyl alcohol
	UN 2937
	alcohol methyl benzylic
	benzyl alcohol, .alpha.-methyl-
	dl-«alpha»-Methylbenzyl alcohol
	dl-Â«alphaÂ»-Methylbenzyl alcohol
	sec-Phenethyl alcohol
	«alpha»-Hydroxyethylbenzene
	«alpha»-Methylbenzenemethanol
	«alpha»-Methylbenzyl alcohol
	«alpha»-Phenethyl alcohol
	«alpha»-Phenylethanol
	«alpha»-Phenylethyl alcohol
	Â«alphaÂ»-Hydroxyethylbenzene
	Â«alphaÂ»-Methylbenzenemethanol
	Â«alphaÂ»-Methylbenzyl alcohol
	Â«alphaÂ»-Phenethyl alcohol
	Â«alphaÂ»-Phenylethanol
	Â«alphaÂ»-Phenylethyl alcohol
Inchi:	InChI=1S/C8H10O/c1-7(9)8-5-3-2-4-6-8/h2-7,9H,1H3
InchiKey:	WAPNOHKVXSQRPX-UHFFFAOYSA-N
Formula:	C8H10O

SMILES: CC(O)c1ccccc1
Mol. weight [g/mol]: 122.16
CAS: 98-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-10.37	kJ/mol	Joback Method
hf	-129.43	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	75.20	kJ/mol	NIST Webbook
log10ws	-0.92		Aqueous Solubility Prediction Method
log10ws	-0.92		Estimated Solubility Method
logp	1.740		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1072.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1033.40		NIST Webbook
rinpol	1027.70		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1038.00		NIST Webbook

rinpol	1051.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	492.60 ± 0.50	K	NIST Webbook
tb	475.65 ± 2.00	K	NIST Webbook
tb	476.55	K	NIST Webbook
tb	476.85	K	NIST Webbook
tc	702.73	K	Joback Method
tf	294.55	K	NIST Webbook

tf	288.00 ± 2.00	K	NIST Webbook
tf	289.82	K	Aqueous Solubility Prediction Method
tf	291.70	K	Energetics and structural properties of neutral and deprotonated phenyl carbinols
tf	293.85	K	NIST Webbook
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.10	J/mol×K	635.44	Joback Method
cpg	254.95	J/mol×K	601.79	Joback Method
cpg	245.20	J/mol×K	568.15	Joback Method
cpg	234.83	J/mol×K	534.50	Joback Method
cpg	223.82	J/mol×K	500.86	Joback Method
cpg	280.74	J/mol×K	702.73	Joback Method
cpg	272.69	J/mol×K	669.08	Joback Method
dvisc	0.0382650	Pa×s	252.16	Joback Method
dvisc	0.0077399	Pa×s	293.61	Joback Method
dvisc	0.0023249	Pa×s	335.06	Joback Method
dvisc	0.0009101	Pa×s	376.51	Joback Method
dvisc	0.0004291	Pa×s	417.96	Joback Method
dvisc	0.0002317	Pa×s	459.41	Joback Method
dvisc	0.0001385	Pa×s	500.86	Joback Method
pvap	0.14	kPa	323.39	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.02	kPa	303.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.02	kPa	303.35	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.02	kPa	303.35	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.04	kPa	313.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water

pvap	0.06	kPa	313.37	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.06	kPa	313.37	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.10	kPa	323.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.15	kPa	323.39	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.14	kPa	323.39	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	9.96e-03	kPa	293.34	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.20	kPa	333.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.26	kPa	333.39	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.26	kPa	333.39	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.40	kPa	343.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	9.95e-03	kPa	293.33	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.52	kPa	343.42	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.76	kPa	353.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.90	kPa	353.43	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.91	kPa	353.43	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water

pvap	1.35	kPa	363.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	1.56	kPa	363.43	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	1.56	kPa	363.43	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	6.00e-03	kPa	293.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	7.33	kPa	398.01	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	5.99	kPa	393.34	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	5.93	kPa	393.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	4.56	kPa	387.28	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	3.73	kPa	382.98	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate

pvap	2.30	kPa	373.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	2.11	kPa	371.46	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	1.61	kPa	366.37	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	1.30	kPa	362.36	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	1.03	kPa	358.41	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	2.91	kPa	377.83	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	0.52	kPa	343.42	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	0.76	kPa	353.15	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate

rfi	1.52250		298.20	Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure	
rhol	996.58	kg/m3	313.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - a-methyl benzyl alcohol - water system	
rhol	1000.73	kg/m3	308.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - a-methyl benzyl alcohol - water system	
rhol	1004.86	kg/m3	303.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - a-methyl benzyl alcohol - water system	
rhol	1009.00	kg/m3	298.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - a-methyl benzyl alcohol - water system	

rhol	1006.48	kg/m3	298.00	Optimization of liquid-liquid equilibria of the type 2 ternary systems (water + valeric acid + aromatic solvent): Modeling through SERLAS
rhol	1006.48	kg/m3	298.20	Optimization and modeling of extraction equilibria of the type 2 ternary systems containing (water + isovaleric acid + solvent)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	477.20	K	99.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98851&Units=SI
High pressure vapour liquid equilibria of the binary and some of the ternary and multicomponent mixtures of the carbon dioxide + acetic anhydride + alpha-methylbenzyl alcohol + acetic acid + alpha-methylbenzyl acetate system: Experimental and modelling results:	https://www.doi.org/10.1016/j.fluid.2006.04.011
Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water:	https://www.doi.org/10.1021/je060157s
Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2007.10.011
Liquid-Liquid Equilibrium for the Ternary System Water + Ethylbenzene + 1-Phenylethanol:	https://www.doi.org/10.1021/je500726x
Phase equilibria of the ternary system + Acetophenone ... dioxide at high pressure conditions:	https://www.doi.org/10.1016/j.fluid.2008.02.010
Energetic and structural properties of neutral and deprotonated phenyl carbinols:	https://www.doi.org/10.1016/j.jct.2016.02.010
Optimization of liquid-liquid equilibria of the type 2 ternary systems (water + valeric acid + aromatic solvent): Modeling through SERLAS:	https://www.doi.org/10.1016/j.fluid.2016.01.050
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - a-methyl benzyl alcohol - water system:	https://www.doi.org/10.1016/j.jct.2013.03.023
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Optimization and modeling of extraction equilibria of the type 2 ternary systems containing (water + isovaleric acid + solvent):	https://www.doi.org/10.1016/j.jct.2015.07.035
Phase equilibria of ternary systems (water + pyruvic acid + high boiling alcohol): Thermodynamic modeling and optimization of extraction:	https://www.doi.org/10.1016/j.jct.2012.06.019
Vapor-Liquid Equilibrium for Phenol and r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate:	https://www.doi.org/10.1021/je025566c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume