

# 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, Ä«alphaÄ»-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-Ä«alphaÄ»-Methylbenzyl alcohol  
sec-Phenethyl alcohol  
«alpha»-Hydroxyethylbenzene  
«alpha»-Methylbenzenemethanol  
«alpha»-Methylbenzyl alcohol  
«alpha»-Phenethyl alcohol  
«alpha»-Phenylethanol  
«alpha»-Phenylethyl alcohol  
Ä«alphaÄ»-Hydroxyethylbenzene  
Ä«alphaÄ»-Methylbenzenemethanol  
Ä«alphaÄ»-Methylbenzyl alcohol  
Ä«alphaÄ»-Phenethyl alcohol  
Ä«alphaÄ»-Phenylethanol  
Ä«alphaÄ»-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	1043.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1029.00		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	1063.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1061.00		NIST Webbook

rinp0	1042.00		NIST Webbook
rip0	1822.00		NIST Webbook
rip0	1777.00		NIST Webbook
rip0	1776.00		NIST Webbook
rip0	1812.00		NIST Webbook
rip0	1827.00		NIST Webbook
rip0	1822.00		NIST Webbook
rip0	1795.00		NIST Webbook
rip0	1822.00		NIST Webbook
rip0	1825.00		NIST Webbook
rip0	1760.00		NIST Webbook
rip0	1805.00		NIST Webbook
rip0	1805.00		NIST Webbook
rip0	1782.00		NIST Webbook
rip0	1765.00		NIST Webbook
rip0	1821.00		NIST Webbook
rip0	1801.00		NIST Webbook
rip0	1819.00		NIST Webbook
rip0	1816.00		NIST Webbook
rip0	1795.00		NIST Webbook
rip0	1782.00		NIST Webbook
rip0	1785.00		NIST Webbook
rip0	1782.00		NIST Webbook
rip0	1773.00		NIST Webbook
rip0	1820.00		NIST Webbook
rip0	1820.00		NIST Webbook
rip0	1820.00		NIST Webbook
rip0	1764.00		NIST Webbook
rip0	1817.00		NIST Webbook
rip0	1813.00		NIST Webbook
rip0	1812.00		NIST Webbook
rip0	1796.00		NIST Webbook
rip0	1785.00		NIST Webbook
rip0	1780.00		NIST Webbook
rip0	1791.00		NIST Webbook
rip0	1818.00		NIST Webbook
rip0	1765.00		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	289.82	K	Aqueous Solubility Prediction Method

tf	294.55	K	NIST Webbook
tf	288.00 ± 2.00	K	NIST Webbook
tf	293.85	K	NIST Webbook
tf	291.70	K	Energetics and structural properties of neutral and deprotonated phenyl carbinols
vc	0.389	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.82	J/mol×K	500.86	Joback Method
cpg	234.83	J/mol×K	534.50	Joback Method
cpg	245.20	J/mol×K	568.15	Joback Method
cpg	254.95	J/mol×K	601.79	Joback Method
cpg	264.10	J/mol×K	635.44	Joback Method
cpg	272.69	J/mol×K	669.08	Joback Method
cpg	280.74	J/mol×K	702.73	Joback Method
dvisc	0.0382650	Paxs	252.16	Joback Method
dvisc	0.0077399	Paxs	293.61	Joback Method
dvisc	0.0023249	Paxs	335.06	Joback Method
dvisc	0.0009101	Paxs	376.51	Joback Method
dvisc	0.0004291	Paxs	417.96	Joback Method
dvisc	0.0002317	Paxs	459.41	Joback Method
dvisc	0.0001385	Paxs	500.86	Joback Method
pvap	0.02	kPa	303.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	1.03	kPa	358.41	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	1.61	kPa	366.37	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	2.30	kPa	373.15	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	3.73	kPa	382.98	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	5.93	kPa	393.15	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	7.33	kPa	398.01	Vapor-Liquid Equilibrium for Phenol + r-Methyl Benzyl Alcohol and 2-Ethoxyethanol + n-Butyl Formate
pvap	6.00e-03	kPa	293.15	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	9.95e-03	kPa	293.33	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water
pvap	9.96e-03	kPa	293.34	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
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	0.14	kPa	323.39	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	1.56	kPa	363.43	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	0.52	kPa	343.42	Vapor-Liquid Equilibrium in r-Methylbenzenemethanol + Water

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	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	1009.00	kg/m3	298.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - $\alpha$ -methyl benzyl alcohol - water system
rhol	1004.86	kg/m3	303.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - $\alpha$ -methyl benzyl alcohol - water system
rhol	1000.73	kg/m3	308.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - $\alpha$ -methyl benzyl alcohol - water system

rhol	996.58	kg/m3	313.15	Experimental density, viscosity, interfacial tension and water solubility of ethyl benzene - $\alpha$ -methyl benzyl alcohol - water system
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

# Legend

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

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