

Benzeneethanol, «alpha»-methyl-

Other names:	«alpha»-Methylphenethyl alcohol Benzyl methyl carbinol Phenethyl alcohol, «alpha»-methyl- 1-Phenyl-2-propanol 2-Hydroxy-1-phenylpropane 2-Propanol, 1-phenyl- «alpha»-Methylbenzeneethanol Benzenethanol, «alpha»-methyl- NSC 53553 1-phenylpropan-2-ol
Inchi:	InChI=1S/C9H12O/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3
InchiKey:	WYTRYIUQUUDTGSX-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CC(O)Cc1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	698-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-1.95	kJ/mol	Joback Method
hf	-150.07	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.610		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
ripol	1212.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1778.00		NIST Webbook
tb	523.74	K	Joback Method
tc	722.83	K	Joback Method
tf	263.43	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.01	J/molxK	523.74	Joback Method
cpg	278.99	J/molxK	556.92	Joback Method
cpg	290.28	J/molxK	590.10	Joback Method
cpg	300.91	J/molxK	623.28	Joback Method
cpg	310.91	J/molxK	656.46	Joback Method
cpg	320.31	J/molxK	689.65	Joback Method
cpg	329.13	J/molxK	722.83	Joback Method
dvisc	0.0307952	Paxs	263.43	Joback Method
dvisc	0.0063252	Paxs	306.81	Joback Method
dvisc	0.0019230	Paxs	350.20	Joback Method
dvisc	0.0007602	Paxs	393.59	Joback Method
dvisc	0.0003613	Paxs	436.97	Joback Method
dvisc	0.0001964	Paxs	480.36	Joback Method
dvisc	0.0001181	Paxs	523.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C698873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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