Benzeneethanol, «beta»-methyl-

Other names:	Phenethyl alcohol, «beta»-methyl-
	«beta»-Methylphenethyl alcohol
	«beta»-Phenylpropyl alcohol
	Hydratropic alcohol
	Hydratropyl alcohol
	1-Propanol, 2-phenyl-
	2-Phenyl-1-propanol
	2-Phenylpropyl alcohol
	1-Hydroxy-2-phenylpropane
	2-Phenylpropan-1-ol
	2-Phenylpropanol
	NSC 5232
	«beta»-Methylphenetyl alcohol
	1-(2-Phenyl)-1-propanol
Inchi:	InChI=1S/C9H12O/c1-8(7-10)9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3
InchiKey:	RNDNSYIPLPAXAZ-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CC(CO)c1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	1123-85-9

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	-1.92		Crippen Method
logp	1.782		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1144.60		NIST Webbook
ripol	1975.10		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1975.10		NIST Webbook
ripol	1920.00		NIST Webbook

tb	523.74	K	Joback Method
tc	722.83	K	Joback Method
tf	263.43	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.70	K	1.30	NIST Webbook
tbrp	389.00 ± 1.00	K	2.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
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