«beta»-Phenylethylmethylethylcarbinol

Other names: Benzenepropanol, «alpha»-ethyl-«alpha»-methyl-
Phenethylmethylethylcarbinol
Phenylethyl methyl ethyl carbinol
3-Pentanol, 3-methyl-1-phenyl-
1-Phenyl-3-methyl-3-pentanol
3-methyl-1-phenylpentan-3-ol
Inchi: InChI=1S/C12H18O/c1-3-12(2,13)10-9-11-7-5-4-6-8-11/h4-8,13H,3,9-10H2,1-2H3
InchiKey: AEJRTNBCFUOSEM-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCC(C)(O)CCc1ccccc1
Mol. weight [g/mol]: 178.27
CAS: 10415-87-9

Physical Properties

Property code	Value	Unit	Source
gf	28.59	kJ/mol	Joback Method
hf	-215.46	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.780		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	589.59	K	Joback Method
tc	787.78	K	Joback Method
tf	314.66	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.15	J/mol×K	589.59	Joback Method
cpg	424.76	J/mol×K	622.62	Joback Method
cpg	438.47	J/mol×K	655.65	Joback Method

cpg	451.33	J/mol×K	688.68	Joback Method
cpg	463.38	J/mol×K	721.71	Joback Method
cpg	474.67	J/mol×K	754.74	Joback Method
cpg	485.26	J/mol×K	787.78	Joback Method
dvisc	0.0112365	Pa×s	314.66	Joback Method
dvisc	0.0028066	Pa×s	360.48	Joback Method
dvisc	0.0009586	Pa×s	406.30	Joback Method
dvisc	0.0004070	Pa×s	452.12	Joback Method
dvisc	0.0002023	Pa×s	497.95	Joback Method
dvisc	0.0001132	Pa×s	543.77	Joback Method
dvisc	0.0000693	Pa×s	589.59	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10415879&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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