Benzeneethanol, «alpha»,«alpha»-dimethyl-

Other names: Phenethyl alcohol, «alpha»,«alpha»-dimethyl-
«alpha»,«alpha»-Dimethylphenethanol
«alpha»,«alpha»-Dimethylphenethyl alcohol
Benzyldimethylcarbinol
Dimethylbenzylcarbinol
DMBC
1,1-Dimethyl-2-Phenylethanol
1,1-Dimethylphenylethanol
2-Methyl-1-phenyl-2-propanol
Phenyl-tert-butanol
«alpha»,«alpha»-Dimethyl-«beta»-phenylethyl alcohol
«beta»-Phenyl-tert-butyl alcohol
2-Benzyl-2-propanol
2-Hydroxy-2-methyl-1-phenylpropane
2-Methyl-3-phenyl-2-propanol
1,1-Dimethyl-2-phenylethyl alcohol
2-Methyl-1-phenylpropan-2-ol
Ethanol, 1,1-dimethyl-2-phenyl-
«alpha»,«alpha»-Dimethylphenylethyl alcohol
NSC 27228

Inchi: InChI=1S/C10H14O/c1-10(2,11)8-9-6-4-3-5-7-9/h3-7,11H,8H2,1-2H3
InchiKey: RIWRBSMFKVOJMN-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC(C)(O)Cc1ccccc1
Mol. weight [g/mol]: 150.22
CAS: 100-86-7

Physical Properties

Property code	Value	Unit	Source
gf	11.75	kJ/mol	Joback Method
hf	-174.18	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.000		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method

rinpol	1124.60		NIST Webbook
ripol	1781.00		NIST Webbook
tb	543.83	K	Joback Method
tc	747.81	K	Joback Method
tf	292.12	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.14	J/mol×K	543.83	Joback Method
cpg	328.48	J/mol×K	577.83	Joback Method
cpg	340.94	J/mol×K	611.82	Joback Method
cpg	352.57	J/mol×K	645.82	Joback Method
cpg	363.42	J/mol×K	679.82	Joback Method
cpg	373.54	J/mol×K	713.82	Joback Method
cpg	382.98	J/mol×K	747.81	Joback Method
dvisc	0.0171729	Pa×s	292.12	Joback Method
dvisc	0.0042551	Pa×s	334.07	Joback Method
dvisc	0.0014394	Pa×s	376.02	Joback Method
dvisc	0.0006053	Pa×s	417.97	Joback Method
dvisc	0.0002981	Pa×s	459.93	Joback Method
dvisc	0.0001653	Pa×s	501.88	Joback Method
dvisc	0.0001003	Pa×s	543.83	Joback Method

Sources

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=C100867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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