Benzenepropanol, «alpha»,«alpha»-dimethyl-

Other names:	1-Propanol, 1,1-dimethyl-3-phenyl-
	Benzyl-tert-butanol
	Dimethylphenethylcarbinol
	Dimethylphenylethylcarbinol
	Phenylethyl dimethyl carbinol
	2-(2-Phenylethyl)-2-propanol
	2-Butanol, 2-methyl-4-phenyl-
	2-Methyl-4-phenyl-2-butanol
	«alpha»,«alpha»-Dimethyl-«gamma»-phenylpropyl alcohol
	1,1-Dimethyl-3-phenyl-1-propanol
	1,1-Dimethyl-3-phenylpropanol
	Benzyl-t-butanol
	1,1-Dimethyl-3-phenylpropyl alcohol
	1-Phenyl-3-methylbutan-3-ol
	2-Phenethyl-2-propanol
	NSC 62145
	2-methyl-4-phenylbutan-2-ol
Inchi:	InChI=1S/C11H16O/c1-11(2,12)9-8-10-6-4-3-5-7-10/h3-7,12H,8-9H2,1-2H3
InchiKey:	YXVSKJDFNJFXAJ-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CC(C)(O)CCc1ccccc1
Mol. weight [g/mol]:	164.24
CAS:	103-05-9

Physical Properties

Property code	Value	Unit	Source
gf	20.17	kJ/mol	Joback Method
hf	-194.82	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	57.74	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.390		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1270.50		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook

ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	566.71	K	Joback Method
tc	767.71	K	Joback Method
tf	303.39	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.84	J/mol×K	566.71	Joback Method
cpg	423.51	J/mol×K	734.21	Joback Method
cpg	412.76	J/mol×K	700.71	Joback Method
cpg	401.27	J/mol×K	667.21	Joback Method
cpg	388.99	J/mol×K	633.71	Joback Method
cpg	375.86	J/mol×K	600.21	Joback Method
cpg	433.56	J/mol×K	767.71	Joback Method
dvisc	0.0000834	Pa×s	566.71	Joback Method
dvisc	0.0001368	Pa×s	522.82	Joback Method
dvisc	0.0002457	Pa×s	478.94	Joback Method
dvisc	0.0004965	Pa×s	435.05	Joback Method
dvisc	0.0011748	Pa×s	391.16	Joback Method
dvisc	0.0034560	Pa×s	347.28	Joback Method
dvisc	0.0138910	Pa×s	303.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	11.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103059&Units=SI

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