Clobutinol

Other names:	Benzeneethanol, 4-chloro-«alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-methyl-
	Phenethyl alcohol, p-chloro-«alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-methyl-
	Benzeneethanol, 4-chloro-«alpha»-(2-(dimethylamino)-1-methyl)-«alpha»-methyl-
	p-Chloro-«alpha»-(2-(dimethylamino)-1-methylethyl)-«alpha»-methyl-phenethyl alcohol
	1-(4-Chlorophenyl)-2,3-dimethyl-4-dimethylamino-2-butanol
	p-Cloro-«alpha»-(2-(dimetilamino)-1-metiletil)-«alpha»-metil fenetil alcool
	p-Chloro-«alpha»-[2-(dimethylamino)-1-methylethyl]-«alpha»-methylphenyl alcohol
Inchi:	InChI=1S/C14H22ClNO/c1-11(10-16(3)4)14(2,17)9-12-5-7-13(15)8-6-12/h5-8,11,17H,9-1
InchiKey:	KVHHQGIIZCJATJ-UHFFFAOYSA-N
Formula:	C14H22ClNO
SMILES:	CC(CN(C)C)C(C)(O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	255.78
CAS:	14860-49-2

Physical Properties

Property code	Value	Unit	Source
gf	132.21	kJ/mol	Joback Method
hf	-221.70	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.831		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	689.76	K	Joback Method
tc	889.00	K	Joback Method
tf	397.11	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.03	J/mol×K	689.76	Joback Method
cpg	593.86	J/mol×K	722.97	Joback Method
cpg	607.76	J/mol×K	756.17	Joback Method
cpg	620.78	J/mol×K	789.38	Joback Method
cpg	632.99	J/mol×K	822.59	Joback Method
cpg	644.44	J/mol×K	855.80	Joback Method
cpg	655.21	J/mol×K	889.00	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=C14860492&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume