

[1,1'-Bicyclohexyl]-2-ol, 5-(1,1-dimethylethyl)-

Other names:	2-Cyclohexyl-4-tert-butyl cyclohexanol
Inchi:	InChI=1S/C16H30O/c1-16(2,3)13-9-10-15(17)14(11-13)12-7-5-4-6-8-12/h12-15,17H,4-11
InchiKey:	MWLJRXJLIWTESD-UHFFFAOYSA-N
Formula:	C16H30O
SMILES:	CC(C)(C)C1CCC(O)C(C2CCCCC2)C1
Mol. weight [g/mol]:	238.41
CAS:	55538-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.66	kJ/mol	Joback Method
hf	-466.59	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	66.83	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.390		Crippen Method
mcvol	220.450	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
tb	684.19	K	Joback Method
tc	895.97	K	Joback Method
tf	339.60	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.31	J/molxK	684.19	Joback Method
cpg	791.26	J/molxK	860.67	Joback Method
cpg	773.71	J/molxK	825.38	Joback Method
cpg	754.80	J/molxK	790.08	Joback Method
cpg	734.47	J/molxK	754.78	Joback Method
cpg	712.66	J/molxK	719.49	Joback Method
cpg	807.51	J/molxK	895.97	Joback Method
dvisc	0.0000525	Paxs	684.19	Joback Method

dvisc	0.0000842	Paxs	626.76	Joback Method
dvisc	0.0001486	Paxs	569.33	Joback Method
dvisc	0.0002980	Paxs	511.90	Joback Method
dvisc	0.0007123	Paxs	454.46	Joback Method
dvisc	0.0021913	Paxs	397.03	Joback Method
dvisc	0.0098572	Paxs	339.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C55538595&Units=SI

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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