

Cyclohexanol,5-(1,1-dimethylethyl)-2-methylene-t

Inchi:	InChI=1S/C11H20O/c1-8-5-6-9(7-10(8)12)11(2,3)4/h9-10,12H,1,5-7H2,2-4H3/t9-,10+/m0
InchiKey:	MKWJZCGGUSWUQL-VHSXEESVSA-N
Formula:	C11H20O
SMILES:	C=C1CCC(C(C)(C)C)CC1O
Mol. weight [g/mol]:	168.28
CAS:	19245-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-22.42	kJ/mol	Joback Method
hf	-313.13	kJ/mol	Joback Method
hfus	12.67	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
ie	9.37 ± 0.05	eV	NIST Webbook
ie	9.37 ± 0.02	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.750		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	554.07	K	Joback Method
tc	750.02	K	Joback Method
tf	293.79	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.06	J/molxK	554.07	Joback Method
cpg	419.26	J/molxK	586.73	Joback Method
cpg	435.53	J/molxK	619.39	Joback Method
cpg	450.89	J/molxK	652.04	Joback Method
cpg	465.38	J/molxK	684.70	Joback Method
cpg	479.03	J/molxK	717.36	Joback Method
cpg	491.87	J/molxK	750.02	Joback Method

dvisc	0.0151885	Paxs	293.79	Joback Method
dvisc	0.0040285	Paxs	337.17	Joback Method
dvisc	0.0014460	Paxs	380.55	Joback Method
dvisc	0.0006401	Paxs	423.93	Joback Method
dvisc	0.0003297	Paxs	467.31	Joback Method
dvisc	0.0001900	Paxs	510.69	Joback Method
dvisc	0.0001194	Paxs	554.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19245706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ie:	Ionization energy
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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