1-Cyclohexene-1-ethanol, 2,6,6-trimethyl-

Other names: «beta»-Cyclohomogeraniol
Inchi: InChI=1S/C11H20O/c1-9-5-4-7-11(2,3)10(9)6-8-12/h12H,4-8H2,1-3H3
InchiKey: JGJFZOVBBGQGOM-UHFFFAOYSA-N
Formula: C11H20O
SMILES: CC1=C(CCO)C(C)(C)CCC1
Mol. weight [g/mol]: 168.28
CAS: 472-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-65.42	kJ/mol	Joback Method
hf	-318.20	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.895		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	1336.60		NIST Webbook
rinpol	1336.60		NIST Webbook
tb	572.17	K	Joback Method
tc	766.66	K	Joback Method
tf	331.63	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.74	J/mol×K	572.17	Joback Method
cpg	412.89	J/mol×K	604.58	Joback Method
cpg	427.28	J/mol×K	637.00	Joback Method
cpg	440.98	J/mol×K	669.41	Joback Method
cpg	454.09	J/mol×K	701.83	Joback Method
cpg	466.68	J/mol×K	734.24	Joback Method

cpg	478.83	J/mol×K	766.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C472651&Units=SI

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