Cyclohexanol, 1-(1-hexenyl)-, (E)-

Other names: 1-[(1E)-1-Hexenyl]cyclohexanol
(E)-1-(1-Hexenyl)cyclohexanol
Inchi: InChI=1S/C12H22O/c1-2-3-4-6-9-12(13)10-7-5-8-11-12/h6,9,13H,2-5,7-8,10-11H2,1H3/b
InchiKey: ICOITBGCXKPDQU-RMKNXTFCSA-N
Formula: C12H22O
SMILES: CCCCC=CC1(O)CCCCC1
Mol. weight [g/mol]: 182.30
CAS: 34678-40-5

Physical Properties

Property code	Value	Unit	Source
gf	12.52	kJ/mol	Joback Method
hf	-256.46	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.428		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	590.09	K	Joback Method
tc	786.32	K	Joback Method
tf	312.02	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.16	J/mol×K	590.09	Joback Method
cpg	464.97	J/mol×K	622.79	Joback Method
cpg	480.86	J/mol×K	655.50	Joback Method
cpg	495.94	J/mol×K	688.20	Joback Method

cpg	510.31	J/mol×K	720.91	Joback Method
cpg	524.07	J/mol×K	753.61	Joback Method
cpg	537.33	J/mol×K	786.32	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=C34678405&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