4-(3-hydroxy-but-1-enyl)-3,5,5-trimethylcyclohex-3

Inchi: InChI=1S/C13H22O3/c1-8(14)5-6-10-9(2)12(16)11(15)7-13(10,3)4/h5-6,8,11-12,14-16H,
InchiKey: HODWUFMHAGVDJY-AATRIKPKSA-N
Formula: C13H22O3
SMILES: CC1=C(C=CC(C)O)C(C)(C)CC(O)C1O
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-259.86	kJ/mol	Joback Method
hf	-592.68	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.392		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	796.67	K	Joback Method
tc	986.11	K	Joback Method
tf	447.25	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.10	J/mol×K	796.67	Joback Method
cpg	616.26	J/mol×K	828.24	Joback Method
cpg	629.10	J/mol×K	859.82	Joback Method
cpg	641.70	J/mol×K	891.39	Joback Method
cpg	654.14	J/mol×K	922.96	Joback Method
cpg	666.50	J/mol×K	954.53	Joback Method
cpg	678.86	J/mol×K	986.11	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=R407086&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