2-(3-Hydroxybut-1-enyl)-2,6,6-trimethylcyclohex-3

Inchi: InChI=1S/C13H20O2/c1-10(14)6-9-13(4)8-5-7-12(2,3)11(13)15/h5-6,8-10,14H,7H2,1-4H
InchiKey: MGSBKWPNOWBJCU-RMKNXTFCSA-N
Formula: C13H20O2
SMILES: CC(O)C=CC1(C)C=CCC(C)(C)C1=O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-87.33	kJ/mol	Joback Method
hf	-367.40	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.485		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
ripol	2140.00		NIST Webbook
ripol	2140.00		NIST Webbook
tb	675.08	K	Joback Method
tc	892.97	K	Joback Method
tf	396.93	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.76	J/mol×K	675.08	Joback Method
cpg	526.16	J/mol×K	711.39	Joback Method
cpg	542.01	J/mol×K	747.71	Joback Method
cpg	557.51	J/mol×K	784.02	Joback Method
cpg	572.85	J/mol×K	820.34	Joback Method
cpg	588.21	J/mol×K	856.65	Joback Method
cpg	603.80	J/mol×K	892.97	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=R302560&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume