3-Hydroxy-1a,3,6,6-tetramethylhexahydro-2-oxacy

Inchi: InChI=1S/C14H22O3/c1-11(2)5-6-14-8-12(14,3)17-13(4,16)7-9(14)10(11)15/h9,16H,5-8H
InchiKey: WIXKMBYZWQMYGA-UHFFFAOYSA-N
Formula: C14H22O3
SMILES: CC1(O)CC2C(=O)C(C)(C)CCC23CC3(C)O1
Mol. weight [g/mol]: 238.32
CAS: 71596-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-157.86	kJ/mol	Joback Method
hf	-527.86	kJ/mol	Joback Method
hfus	10.75	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.269		Crippen Method
mcvol	188.850	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	727.05	K	Joback Method
tc	960.59	K	Joback Method
tf	537.05	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.88	J/mol×K	727.05	Joback Method
cpg	621.94	J/mol×K	765.97	Joback Method
cpg	641.47	J/mol×K	804.90	Joback Method
cpg	662.00	J/mol×K	843.82	Joback Method
cpg	684.00	J/mol×K	882.74	Joback Method
cpg	707.99	J/mol×K	921.67	Joback Method

cpg	734.47	J/mol×K	960.59	Joback Method

Sources

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=C71596913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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