2,5,5,8a-Tetramethyl-6,7,8,8a-tetrahydro-5H-chron

Inchi: InChI=1S/C13H20O2/c1-9-5-6-10-12(2,3)8-7-11(14)13(10,4)15-9/h5-6,11,14H,7-8H2,1-4
InchiKey: KHKXQUICDUBJND-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC=C2C(C)(C)CCC(O)C2(C)O1
Mol. weight [g/mol]: 208.30
CAS: 97306-62-2

Physical Properties

Property code	Value	Unit	Source
gf	-69.29	kJ/mol	Joback Method
hf	-372.16	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.786		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
tb	650.62	K	Joback Method
tc	866.38	K	Joback Method
tf	415.58	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.21	J/mol×K	650.62	Joback Method
cpg	511.46	J/mol×K	686.58	Joback Method
cpg	527.05	J/mol×K	722.54	Joback Method
cpg	542.16	J/mol×K	758.50	Joback Method
cpg	557.03	J/mol×K	794.46	Joback Method
cpg	571.84	J/mol×K	830.42	Joback Method
cpg	586.83	J/mol×K	866.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97306622&Units=SI
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

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