5-Hydroxy-2,2,6,6-tetramethyl-4-propionylcyclohe

Inchi: InChI=1S/C13H18O4/c1-6-7(14)8-9(15)12(2,3)11(17)13(4,5)10(8)16/h15H,6H2,1-5H3
InchiKey: KHGAQCGCKVOTAB-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CCC(=O)C1=C(O)C(C)(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]: 238.28
CAS: 87552-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-435.88	kJ/mol	Joback Method
hf	-752.56	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.982		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1464.40		NIST Webbook
rinpol	1464.40		NIST Webbook
tb	803.01	K	Joback Method
tc	1027.18	K	Joback Method
tf	560.20	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.51	J/mol×K	803.01	Joback Method
cpg	594.68	J/mol×K	840.37	Joback Method
cpg	610.80	J/mol×K	877.73	Joback Method
cpg	627.02	J/mol×K	915.09	Joback Method
cpg	643.47	J/mol×K	952.46	Joback Method
cpg	660.30	J/mol×K	989.82	Joback Method
cpg	677.65	J/mol×K	1027.18	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=C87552010&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