Hexanoic acid, 3-hydroxy-2,2-dimethyl-, beta-lactone

Inchi: InChI=1S/C8H14O2/c1-4-5-6-8(2,3)7(9)10-6/h6H,4-5H2,1-3H3
InchiKey: HTONSGUIJYZFOJ-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCCC1OC(=O)C1(C)C
Mol. weight [g/mol]: 142.20
CAS: 90112-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-156.78	kJ/mol	Joback Method
hf	-416.61	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	40.78	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.738		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	483.79	K	Joback Method
tc	695.26	K	Joback Method
tf	308.79	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.23	J/mol×K	483.79	Joback Method
cpg	294.03	J/mol×K	519.03	Joback Method
cpg	308.00	J/mol×K	554.28	Joback Method
cpg	321.22	J/mol×K	589.52	Joback Method
cpg	333.76	J/mol×K	624.77	Joback Method
cpg	345.71	J/mol×K	660.01	Joback Method
cpg	357.14	J/mol×K	695.26	Joback Method

Sources

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=C90112826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume