Heptanoic acid, 2,2,4-trimethyl-3-hydroxy-, beta-lactone

Inchi: InChI=1S/C10H18O2/c1-5-6-7(2)8-10(3,4)9(11)12-8/h7-8H,5-6H2,1-4H3
InchiKey: YQQGTMIMGKGIMY-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCC(C)C1OC(=O)C1(C)C
Mol. weight [g/mol]: 170.25
CAS: 18523-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-142.38	kJ/mol	Joback Method
hf	-463.17	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.374		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
tb	529.11	K	Joback Method
tc	738.85	K	Joback Method
tf	316.33	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.36	J/mol×K	529.11	Joback Method
cpg	387.30	J/mol×K	564.07	Joback Method
cpg	403.34	J/mol×K	599.02	Joback Method
cpg	418.57	J/mol×K	633.98	Joback Method
cpg	433.06	J/mol×K	668.94	Joback Method
cpg	446.91	J/mol×K	703.89	Joback Method
cpg	460.20	J/mol×K	738.85	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=C18523609&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume