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

Inchi: InChI=1S/C8H14O2/c1-5(2)6-8(3,4)7(9)10-6/h5-6H,1-4H3
InchiKey: JMHWSGPTHJGHMB-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CC(C)C1OC(=O)C1(C)C
Mol. weight [g/mol]: 142.20
CAS: 7227-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-159.22	kJ/mol	Joback Method
hf	-421.89	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.594		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	483.35	K	Joback Method
tc	699.79	K	Joback Method
tf	293.79	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.41	J/mol×K	483.35	Joback Method
cpg	294.65	J/mol×K	519.42	Joback Method
cpg	309.00	J/mol×K	555.50	Joback Method
cpg	322.56	J/mol×K	591.57	Joback Method
cpg	335.40	J/mol×K	627.64	Joback Method
cpg	347.62	J/mol×K	663.71	Joback Method
cpg	359.30	J/mol×K	699.79	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=C7227965&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