Hexanoic acid, 5-hydroxy-3-methyl-, «delta»-lactone

Other names: 2H-Pyran-2-one, tetrahydro-4,6-dimethyl-
Inchi: InChI=1S/C7H12O2/c1-5-3-6(2)9-7(8)4-5/h5-6H,3-4H2,1-2H3
InchiKey: KSFJZYURRNSMGO-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC1CC(=O)OC(C)C1
Mol. weight [g/mol]: 128.17
CAS: 3720-20-5

Physical Properties

Property code	Value	Unit	Source
gf	-183.91	kJ/mol	Joback Method
hf	-423.53	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	40.05	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.348		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
ripol	1780.00		NIST Webbook
tb	469.21	K	Joback Method
tc	691.39	K	Joback Method
tf	266.58	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.42	J/mol×K	469.21	Joback Method
cpg	250.08	J/mol×K	506.24	Joback Method
cpg	265.11	J/mol×K	543.27	Joback Method
cpg	279.49	J/mol×K	580.30	Joback Method
cpg	293.21	J/mol×K	617.33	Joback Method
cpg	306.23	J/mol×K	654.36	Joback Method
cpg	318.55	J/mol×K	691.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3720205&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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