4,5-dihydroxy-hexanoic acid lactone

Inchi: InChI=1S/C6H10O3/c1-4-5(7)2-3-6(8)9-4/h4-5,7H,2-3H2,1H3
InchiKey: SRADPKRSAISFSJ-UHFFFAOYSA-N
Formula: C6H10O3
SMILES: CC1OC(=O)CCC1O
Mol. weight [g/mol]: 130.14

Physical Properties

Property code	Value	Unit	Source
gf	-329.15	kJ/mol	Joback Method
hf	-555.12	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	54.51	kJ/mol	Joback Method
log10ws	-0.58		Crippen Method
logp	0.073		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	538.51	K	Joback Method
tc	748.29	K	Joback Method
tf	316.13	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.18	J/mol×K	538.51	Joback Method
cpg	255.59	J/mol×K	573.47	Joback Method
cpg	267.46	J/mol×K	608.44	Joback Method
cpg	278.77	J/mol×K	643.40	Joback Method
cpg	289.50	J/mol×K	678.37	Joback Method
cpg	299.63	J/mol×K	713.33	Joback Method

cpg	309.15	J/mol×K	748.29	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=R489835&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume