[4,4,6,6,6-2H5]Mevalonic Acid Lactone

Inchi: InChI=1S/C6H10O3/c1-6(8)2-3-9-5(7)4-6/h8H,2-4H2,1H3/t6-/m1/s1/i1D3,2D2
InchiKey: JYVXNLLUYHCIIH-WBKASDIDSA-N
Formula: C6H5D5O3
SMILES: CC1(O)CCOC(=O)C1
Mol. weight [g/mol]: 135.17

Physical Properties

Property code	Value	Unit	Source
gf	-326.93	kJ/mol	Joback Method
hf	-519.54	kJ/mol	Joback Method
hfus	8.41	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.074		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	543.42	K	Joback Method
tc	761.96	K	Joback Method
tf	344.27	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.76	J/mol×K	543.42	Joback Method
cpg	252.38	J/mol×K	579.84	Joback Method
cpg	263.36	J/mol×K	616.27	Joback Method
cpg	273.77	J/mol×K	652.69	Joback Method
cpg	283.68	J/mol×K	689.11	Joback Method
cpg	293.16	J/mol×K	725.54	Joback Method
cpg	302.30	J/mol×K	761.96	Joback Method

Sources

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=R412429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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