N-Hexanoyl-DL-homoserine lactone

Inchi: InChI=1S/C10H17NO3/c1-2-3-4-5-9(12)11-8-6-7-14-10(8)13/h8H,2-7H2,1H3,(H,11,12)
InchiKey: ZJFKKPDLNLCPNP-UHFFFAOYSA-N
Formula: C10H17NO3
SMILES: CCCCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 199.25
CAS: 106983-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-178.37	kJ/mol	Joback Method
hf	-518.06	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	0.998		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1741.50		NIST Webbook
tb	642.29	K	Joback Method
tc	854.30	K	Joback Method
tf	410.74	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.44	J/mol×K	642.29	Joback Method
cpg	461.12	J/mol×K	677.62	Joback Method
cpg	475.90	J/mol×K	712.96	Joback Method
cpg	489.77	J/mol×K	748.29	Joback Method
cpg	502.75	J/mol×K	783.63	Joback Method
cpg	514.84	J/mol×K	818.96	Joback Method
cpg	526.04	J/mol×K	854.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106983282&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume