N-Decanoyl-DL-homoserine lactone

Inchi: InChI=1S/C14H25NO3/c1-2-3-4-5-6-7-8-9-13(16)15-12-10-11-18-14(12)17/h12H,2-11H2
InchiKey: TZWZKDULKILUPV-UHFFFAOYSA-N
Formula: C14H25NO3
SMILES: CCCCCCCCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 255.35
CAS: 106983-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-144.69	kJ/mol	Joback Method
hf	-600.62	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.559		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2169.10		NIST Webbook
rinpol	2169.10		NIST Webbook
tb	733.81	K	Joback Method
tc	935.20	K	Joback Method
tf	455.82	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.04	J/mol×K	733.81	Joback Method
cpg	678.23	J/mol×K	767.37	Joback Method
cpg	694.37	J/mol×K	800.94	Joback Method
cpg	709.48	J/mol×K	834.50	Joback Method
cpg	723.57	J/mol×K	868.07	Joback Method
cpg	736.67	J/mol×K	901.63	Joback Method
cpg	748.78	J/mol×K	935.20	Joback Method

Sources

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=C106983362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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