N-Dodecanoyl-DL-homoserine lactone

Inchi: InChI=1S/C16H29NO3/c1-2-3-4-5-6-7-8-9-10-11-15(18)17-14-12-13-20-16(14)19/h14H,2
InchiKey: WILLZMOKUUPJSL-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: CCCCCCCCCCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 283.41
CAS: 18627-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-127.85	kJ/mol	Joback Method
hf	-641.90	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.339		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2384.80		NIST Webbook
tb	779.57	K	Joback Method
tc	978.40	K	Joback Method
tf	478.36	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.67	J/mol×K	779.57	Joback Method
cpg	793.29	J/mol×K	812.71	Joback Method
cpg	809.81	J/mol×K	845.85	Joback Method
cpg	825.23	J/mol×K	878.98	Joback Method
cpg	839.58	J/mol×K	912.12	Joback Method
cpg	852.89	J/mol×K	945.26	Joback Method
cpg	865.17	J/mol×K	978.40	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=C18627388&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