N-Tetradecanoyl-DL-homoserine lactone

Inchi: InChI=1S/C18H33NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17(20)19-16-14-15-22-18(16)21/h
InchiKey: ZQAYHOXXVBVXPZ-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: CCCCCCCCCCCCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 311.46
CAS: 98206-80-5

Physical Properties

Property code	Value	Unit	Source
gf	-111.01	kJ/mol	Joback Method
hf	-683.18	kJ/mol	Joback Method
hfus	50.50	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.119		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2598.60		NIST Webbook
rinpol	2598.60		NIST Webbook
tb	825.33	K	Joback Method
tc	1023.92	K	Joback Method
tf	500.90	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.98	J/mol×K	825.33	Joback Method
cpg	911.95	J/mol×K	858.43	Joback Method
cpg	928.75	J/mol×K	891.53	Joback Method
cpg	944.38	J/mol×K	924.62	Joback Method
cpg	958.89	J/mol×K	957.72	Joback Method
cpg	972.30	J/mol×K	990.82	Joback Method
cpg	984.62	J/mol×K	1023.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98206805&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

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