N-Capryloyl-DL-homoserine lactone

Inchi: InChI=1S/C12H21NO3/c1-2-3-4-5-6-7-11(14)13-10-8-9-16-12(10)15/h10H,2-9H2,1H3,(H
InchiKey: JKEJEOJPJVRHMQ-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCCCCCCC(=O)NC1CCOC1=O
Mol. weight [g/mol]: 227.30
CAS: 106983-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-161.53	kJ/mol	Joback Method
hf	-559.34	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.779		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1958.90		NIST Webbook
rinpol	1958.90		NIST Webbook
tb	688.05	K	Joback Method
tc	893.95	K	Joback Method
tf	433.28	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.73	J/mol×K	688.05	Joback Method
cpg	567.31	J/mol×K	722.37	Joback Method
cpg	582.90	J/mol×K	756.68	Joback Method
cpg	597.52	J/mol×K	791.00	Joback Method
cpg	611.18	J/mol×K	825.32	Joback Method
cpg	623.89	J/mol×K	859.63	Joback Method
cpg	635.67	J/mol×K	893.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106983306&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