N-Z-L-Homoserine lactone

Inchi: InChI=1S/C12H13NO4/c14-11-10(6-7-16-11)13-12(15)17-8-9-4-2-1-3-5-9/h1-5,10H,6-8H
InchiKey: FKWDZIFOVOUDAG-UHFFFAOYSA-N
Formula: C12H13NO4
SMILES: O=C(NC1CCOC1=O)OCc1ccccc1
Mol. weight [g/mol]: 235.24
CAS: 35677-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-154.12	kJ/mol	Joback Method
hf	-455.03	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.228		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	2099.50		NIST Webbook
tb	737.15	K	Joback Method
tc	979.61	K	Joback Method
tf	481.93	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.60	J/mol×K	737.15	Joback Method
cpg	507.47	J/mol×K	777.56	Joback Method
cpg	521.04	J/mol×K	817.97	Joback Method
cpg	533.31	J/mol×K	858.38	Joback Method
cpg	544.30	J/mol×K	898.79	Joback Method
cpg	554.02	J/mol×K	939.20	Joback Method
cpg	562.47	J/mol×K	979.61	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=C35677895&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