

L-Homoserine lactone, N-acetyl-

Inchi:	InChI=1S/C6H9NO3/c1-4(8)7-5-2-3-10-6(5)9/h5H,2-3H2,1H3,(H,7,8)
InchiKey:	XGSXMDQVYYCSDA-UHFFFAOYSA-N
Formula:	C6H9NO3
SMILES:	CC(O)=NC1CCOC1=O
Mol. weight [g/mol]:	143.14

Physical Properties

Property code	Value	Unit	Source
hf	-456.19	kJ/mol	Joback Method
hvap	58.04	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	0.278		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	615.47	K	Joback Method
tc	837.82	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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

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