

# N-Z-L-Homoserine lactone

<b>Inchi:</b>	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
<b>InchiKey:</b>	FKWDZIFOVOUDAG-UHFFFAOYSA-N
<b>Formula:</b>	C12H13NO4
<b>SMILES:</b>	O=C(NC1CCOC1=O)OCc1ccccc1
<b>Mol. weight [g/mol]:</b>	235.24
<b>CAS:</b>	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	m <sup>3</sup> /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

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35677895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35677895&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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