

# N-l-benzoyl lysine

<b>Inchi:</b>	InChI=1S/C13H18N2O3/c14-11(13(17)18)8-4-5-9-15-12(16)10-6-2-1-3-7-10/h1-3,6-7,11H
<b>InchiKey:</b>	KODLJWKGAKBGOB-UHFFFAOYSA-N
<b>Formula:</b>	C13H18N2O3
<b>SMILES:</b>	NC(CCCNC(=O)c1ccccc1)C(=O)O
<b>Mol. weight [g/mol]:</b>	250.29
<b>CAS:</b>	5107-18-6

## Physical Properties

Property code	Value	Unit	Source
gf	-70.27	kJ/mol	Joback Method
hf	-370.53	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	0.999		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	845.70	K	Joback Method
tc	1057.70	K	Joback Method
tf	544.29	K	Joback Method
vc	0.745	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.62	J/molxK	845.70	Joback Method
cpg	611.30	J/molxK	881.03	Joback Method
cpg	621.16	J/molxK	916.37	Joback Method
cpg	630.28	J/molxK	951.70	Joback Method
cpg	638.68	J/molxK	987.03	Joback Method
cpg	646.42	J/molxK	1022.37	Joback Method
cpg	653.55	J/molxK	1057.70	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=C5107186&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5107186&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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