

# 2-Acetylamino-octanoic acid methyl ester

<b>Inchi:</b>	InChI=1S/C11H21NO3/c1-4-5-6-7-8-10(11(14)15-3)12-9(2)13/h10H,4-8H2,1-3H3,(H,12,1
<b>InchiKey:</b>	HXEHVYHMGGXHQE-UHFFFAOYSA-N
<b>Formula:</b>	C11H21NO3
<b>SMILES:</b>	CCCCCCC(NC(C)=O)C(=O)OC
<b>Mol. weight [g/mol]:</b>	215.29

## Physical Properties

Property code	Value	Unit	Source
gf	-234.15	kJ/mol	Joback Method
hf	-579.56	kJ/mol	Joback Method
hfus	30.21	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.635		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpola	1539.00		NIST Webbook
rinpola	1539.00		NIST Webbook
tb	630.97	K	Joback Method
tc	815.25	K	Joback Method
tf	373.48	K	Joback Method
vc	0.711	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.58	J/molxK	630.97	Joback Method
cpg	506.86	J/molxK	661.68	Joback Method
cpg	520.46	J/molxK	692.40	Joback Method
cpg	533.37	J/molxK	723.11	Joback Method
cpg	545.62	J/molxK	753.82	Joback Method
cpg	557.21	J/molxK	784.54	Joback Method
cpg	568.15	J/molxK	815.25	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=R247691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R247691&amp;Units=SI</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>hvpap:</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>rinppl:</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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