

# N-(2-methoxy-5-nitrophenyl)acetamide

<b>Inchi:</b>	InChI=1S/C9H10N2O4/c1-6(12)10-8-5-7(11(13)14)3-4-9(8)15-2/h3-5H,1-2H3,(H,10,12)
<b>InchiKey:</b>	LNEITKYWXMCTLP-UHFFFAOYSA-N
<b>Formula:</b>	C9H10N2O4
<b>SMILES:</b>	COc1ccc([N+](=O)[O-])cc1NC(C)=O
<b>Mol. weight [g/mol]:</b>	210.19
<b>CAS:</b>	33721-54-9

## Physical Properties

Property code	Value	Unit	Source
gf	9.07	kJ/mol	Joback Method
hf	-217.59	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	71.41	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.562		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	720.26	K	Joback Method
tc	960.57	K	Joback Method
tf	511.08	K	Joback Method
vc	0.573	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.70	J/molxK	720.26	Joback Method
cpg	401.69	J/molxK	760.31	Joback Method
cpg	411.81	J/molxK	800.36	Joback Method
cpg	421.07	J/molxK	840.41	Joback Method
cpg	429.48	J/molxK	880.46	Joback Method
cpg	437.05	J/molxK	920.51	Joback Method
cpg	443.81	J/molxK	960.57	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=C33721549&amp;Units=SI&amp;Mask=3FFF">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33721549&amp;Units=SI&amp;Mask=3FFF</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>h vap:</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>m cvol:</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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