

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

Inchi:	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)
InchiKey:	LNEITKYWXMCTLP-UHFFFAOYSA-N
Formula:	C9H10N2O4
SMILES:	COc1ccc([N+](=O)[O-])cc1NC(C)=O
Mol. weight [g/mol]:	210.19
CAS:	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33721549&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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