Acetamide, N-(3-nitrophenyl)-2-methoxy-

Inchi: InChI=1S/C9H10N2O4/c1-15-6-9(12)10-7-3-2-4-8(5-7)11(13)14/h2-5H,6H2,1H3,(H,10,12
InchiKey: SDMUCJMMXQIJMS-UHFFFAOYSA-N
Formula: C9H10N2O4
SMILES: COCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 210.19

Physical Properties

Property code	Value	Unit	Source
gf	18.70	kJ/mol	Joback Method
hf	-206.12	kJ/mol	Joback Method
hfus	31.96	kJ/mol	Joback Method
hvap	70.75	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.180		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	715.28	K	Joback Method
tc	954.78	K	Joback Method
tf	498.56	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.33	J/mol×K	715.28	Joback Method
cpg	403.45	J/mol×K	755.20	Joback Method
cpg	413.66	J/mol×K	795.11	Joback Method
cpg	423.00	J/mol×K	835.03	Joback Method
cpg	431.47	J/mol×K	874.95	Joback Method
cpg	439.11	J/mol×K	914.87	Joback Method
cpg	445.94	J/mol×K	954.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307262&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume