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

Inchi: InChI=1S/C9H10ClNO2/c1-13-6-9(12)11-8-4-2-3-7(10)5-8/h2-5H,6H2,1H3,(H,11,12)
InchiKey: WFOKHEMHRLYTDD-UHFFFAOYSA-N
Formula: C9H10ClNO2
SMILES: COCC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 199.63

Physical Properties

Property code	Value	Unit	Source
gf	-28.78	kJ/mol	Joback Method
hf	-211.10	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.925		Crippen Method
mcvol	143.570	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	600.87	K	Joback Method
tc	822.23	K	Joback Method
tf	384.87	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.59	J/mol×K	600.87	Joback Method
cpg	337.21	J/mol×K	637.76	Joback Method
cpg	348.09	J/mol×K	674.66	Joback Method
cpg	358.25	J/mol×K	711.55	Joback Method
cpg	367.72	J/mol×K	748.44	Joback Method
cpg	376.50	J/mol×K	785.34	Joback Method
cpg	384.60	J/mol×K	822.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307258&Units=SI
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

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