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

Inchi: InChI=1S/C8H7ClN2O3/c9-5-8(12)10-6-2-1-3-7(4-6)11(13)14/h1-4H,5H2,(H,10,12)
InchiKey: UCBHRCPNMDOUMV-UHFFFAOYSA-N
Formula: C8H7ClN2O3
SMILES: O=C(CCl)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 214.61

Physical Properties

Property code	Value	Unit	Source
gf	103.35	kJ/mol	Joback Method
hf	-69.00	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.772		Crippen Method
mcvol	141.030	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1870.00		NIST Webbook
tb	707.41	K	Joback Method
tc	958.39	K	Joback Method
tf	494.98	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.47	J/mol×K	707.41	Joback Method
cpg	350.01	J/mol×K	749.24	Joback Method
cpg	358.68	J/mol×K	791.07	Joback Method
cpg	366.55	J/mol×K	832.90	Joback Method
cpg	373.66	J/mol×K	874.73	Joback Method
cpg	380.06	J/mol×K	916.56	Joback Method
cpg	385.80	J/mol×K	958.39	Joback Method

Sources

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=U307241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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