4-Chloro-3-nitrophenylacetamide

Other names: «alpha»-(4-Chloro-3-nitrophenyl)acetamide
Acetamide, N-(4-chloro-3-nitrophenyl)-
N-(4-chloro-3-nitrophenyl)acetamide
Inchi: InChI=1S/C8H7ClN2O3/c9-6-2-1-5(4-8(10)12)3-7(6)11(13)14/h1-3H,4H2,(H2,10,12)
InchiKey: FPLQCHARENUDSW-UHFFFAOYSA-N
Formula: C8H7ClN2O3
SMILES: NC(=O)Cc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 214.61
CAS: 5540-60-3

Physical Properties

Property code	Value	Unit	Source
gf	70.78	kJ/mol	Joback Method
hf	-100.15	kJ/mol	Joback Method
hfus	32.09	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.276		Crippen Method
mcvol	141.030	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	734.75	K	Joback Method
tc	994.75	K	Joback Method
tf	538.10	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.90	J/mol×K	734.75	Joback Method
cpg	352.90	J/mol×K	778.08	Joback Method
cpg	361.07	J/mol×K	821.42	Joback Method
cpg	368.45	J/mol×K	864.75	Joback Method
cpg	375.10	J/mol×K	908.08	Joback Method
cpg	381.05	J/mol×K	951.41	Joback Method

cpg	386.34	J/mol×K	994.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5540603&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume