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

Inchi: InChI=1S/C9H9ClN2O3/c1-6(10)9(13)11-7-3-2-4-8(5-7)12(14)15/h2-6H,1H3,(H,11,13)
InchiKey: DKFBWJTZPPJWFC-UHFFFAOYSA-N
Formula: C9H9ClN2O3
SMILES: CC(Cl)C(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 228.63

Physical Properties

Property code	Value	Unit	Source
gf	109.33	kJ/mol	Joback Method
hf	-94.92	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	72.34	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.161		Crippen Method
mcvol	155.120	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1873.00		NIST Webbook
tb	729.85	K	Joback Method
tc	980.32	K	Joback Method
tf	491.25	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.51	J/mol×K	729.85	Joback Method
cpg	400.97	J/mol×K	771.60	Joback Method
cpg	410.49	J/mol×K	813.34	Joback Method
cpg	419.13	J/mol×K	855.09	Joback Method
cpg	426.94	J/mol×K	896.83	Joback Method
cpg	433.97	J/mol×K	938.58	Joback Method
cpg	440.29	J/mol×K	980.32	Joback Method

Sources

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=U307489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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