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

Inchi: InChI=1S/C9H9Cl2NO/c1-6(10)9(13)12-8-4-2-3-7(11)5-8/h2-6H,1H3,(H,12,13)
InchiKey: RMICMLBMAQRUJI-UHFFFAOYSA-N
Formula: C9H9Cl2NO
SMILES: CC(Cl)C(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 218.08

Physical Properties

Property code	Value	Unit	Source
gf	61.85	kJ/mol	Joback Method
hf	-99.90	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	60.13	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.906		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
tb	615.44	K	Joback Method
tc	848.25	K	Joback Method
tf	377.56	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.46	J/mol×K	615.44	Joback Method
cpg	337.64	J/mol×K	654.24	Joback Method
cpg	347.98	J/mol×K	693.04	Joback Method
cpg	357.52	J/mol×K	731.84	Joback Method
cpg	366.32	J/mol×K	770.65	Joback Method
cpg	374.39	J/mol×K	809.45	Joback Method
cpg	381.80	J/mol×K	848.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307485&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