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

Inchi: InChI=1S/C8H7Cl2NO/c9-5-8(12)11-7-3-1-2-6(10)4-7/h1-4H,5H2,(H,11,12)
InchiKey: KNVBYGNINQITJC-UHFFFAOYSA-N
Formula: C8H7Cl2NO
SMILES: O=C(CCl)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 204.05

Physical Properties

Property code	Value	Unit	Source
gf	55.87	kJ/mol	Joback Method
hf	-73.98	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.517		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1612.00		NIST Webbook
tb	593.00	K	Joback Method
tc	825.45	K	Joback Method
tf	381.29	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.22	J/mol×K	593.00	Joback Method
cpg	290.21	J/mol×K	631.74	Joback Method
cpg	299.45	J/mol×K	670.48	Joback Method
cpg	307.97	J/mol×K	709.22	Joback Method
cpg	315.83	J/mol×K	747.96	Joback Method
cpg	323.04	J/mol×K	786.71	Joback Method
cpg	329.65	J/mol×K	825.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307237&Units=SI

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