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

Inchi: InChI=1S/C8H6Cl3NO/c9-5-2-1-3-6(4-5)12-8(13)7(10)11/h1-4,7H,(H,12,13)
InchiKey: LCMVVAIGAFVRAL-UHFFFAOYSA-N
Formula: C8H6Cl3NO
SMILES: O=C(Nc1cccc(Cl)c1)C(Cl)Cl
Mol. weight [g/mol]: 238.50

Physical Properties

Property code	Value	Unit	Source
gf	41.50	kJ/mol	Joback Method
hf	-95.00	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	62.29	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.082		Crippen Method
mcvol	148.090	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	629.99	K	Joback Method
tc	870.93	K	Joback Method
tf	396.21	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.74	J/mol×K	629.99	Joback Method
cpg	311.05	J/mol×K	670.15	Joback Method
cpg	319.57	J/mol×K	710.30	Joback Method
cpg	327.35	J/mol×K	750.46	Joback Method
cpg	334.43	J/mol×K	790.62	Joback Method
cpg	340.86	J/mol×K	830.77	Joback Method
cpg	346.68	J/mol×K	870.93	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=U307299&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