3-(2,3-Dichlorophenyl)-1,1-dimethylurea

Other names: Urea, N'-(2,3-dichlorophenyl)-N,N-dimethyl-
1-(2,3-Dichlorophenyl)-3,3-dimethyl urea
Inchi: InChI=1S/C9H10Cl2N2O/c1-13(2)9(14)12-7-5-3-4-6(10)8(7)11/h3-5H,1-2H3,(H,12,14)
InchiKey: ZVPQMESWKIQHGS-UHFFFAOYSA-N
Formula: C9H10Cl2N2O
SMILES: CN(C)C(=O)Nc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 233.09
CAS: 10290-37-6

Physical Properties

Property code	Value	Unit	Source
gf	165.44	kJ/mol	Joback Method
hf	-38.56	kJ/mol	Joback Method
hfus	30.44	kJ/mol	Joback Method
hvap	63.22	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.087		Crippen Method
mcvol	159.920	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	633.30	K	Joback Method
tc	858.57	K	Joback Method
tf	437.55	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.37	J/mol×K	633.30	Joback Method
cpg	371.57	J/mol×K	670.85	Joback Method
cpg	381.95	J/mol×K	708.39	Joback Method
cpg	391.57	J/mol×K	745.94	Joback Method
cpg	400.45	J/mol×K	783.48	Joback Method
cpg	408.65	J/mol×K	821.03	Joback Method
cpg	416.20	J/mol×K	858.57	Joback Method

Sources

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=C10290376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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