N,N'-(Di-3,4-dichlorophenyl)urea

Inchi: InChI=1S/C13H8Cl4N2O/c14-9-3-1-7(5-11(9)16)18-13(20)19-8-2-4-10(15)12(17)6-8/h1-6
InchiKey: ZDPIZPXVHVYTOK-UHFFFAOYSA-N
Formula: C13H8Cl4N2O
SMILES: O=C(Nc1ccc(Cl)c(Cl)c1)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 350.03
CAS: 4300-43-0

Physical Properties

Property code	Value	Unit	Source
gf	247.02	kJ/mol	Joback Method
hf	46.93	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.944		Crippen Method
mcvol	217.000	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	874.05	K	Joback Method
tc	1130.24	K	Joback Method
tf	614.12	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.47	J/mol×K	874.05	Joback Method
cpg	522.85	J/mol×K	916.75	Joback Method
cpg	530.34	J/mol×K	959.45	Joback Method
cpg	537.00	J/mol×K	1002.14	Joback Method
cpg	542.90	J/mol×K	1044.84	Joback Method
cpg	548.10	J/mol×K	1087.54	Joback Method
cpg	552.68	J/mol×K	1130.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4300430&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume