

Urea, N-(2-chlorophenyl)-N'-methyl-

Other names:	Urea, 1-(o-chlorophenyl)-3-methyl- N-Methyl-N1-(2-chlorophenyl)urea 1-(2-Chlorophenyl)-3-methylurea 1-Methyl-3-(2-chlorophenyl)urea
Inchi:	InChI=1S/C8H9ClN2O/c1-10-8(12)11-7-5-3-2-4-6(7)9/h2-5H,1H3,(H2,10,11,12)
InchiKey:	NFUCGJBURDOBPQ-UHFFFAOYSA-N
Formula:	C8H9ClN2O
SMILES:	CNC(=O)Nc1ccccc1Cl
Mol. weight [g/mol]:	184.62
CAS:	15500-96-6

Physical Properties

Property code	Value	Unit	Source
gf	157.19	kJ/mol	Joback Method
hf	-4.77	kJ/mol	Joback Method
hfus	26.12	kJ/mol	Joback Method
hvap	60.34	kJ/mol	Joback Method
ie	8.35 ± 0.05	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	2.091		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	605.74	K	Joback Method
tc	833.08	K	Joback Method
tf	404.03	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.53	J/mol×K	605.74	Joback Method
cpg	312.42	J/mol×K	643.63	Joback Method
cpg	322.53	J/mol×K	681.52	Joback Method
cpg	331.91	J/mol×K	719.41	Joback Method

cpg	340.57	J/mol×K	757.30	Joback Method
cpg	348.56	J/mol×K	795.19	Joback Method
cpg	355.91	J/mol×K	833.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15500966&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
ie:	Ionization energy
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

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