

Urea, (4-chlorophenyl)-

Other names:	Urea, (p-chlorophenyl)- (p-Chlorophenyl)urea p-CPU 4-Chlorophenylurea Urea, 1-(p-chlorophenyl)- 1-(p-Chlorophenyl)urea N-(4-chlorophenyl)urea
Inchi:	InChI=1S/C7H7ClN2O/c8-5-1-3-6(4-2-5)10-7(9)11/h1-4H,(H3,9,10,11)
InchiKey:	RECCURWJDVZHIH-UHFFFAOYSA-N
Formula:	C7H7ClN2O
SMILES:	NC(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	170.60
CAS:	140-38-5

Physical Properties

Property code	Value	Unit	Source
gf	125.83	kJ/mol	Joback Method
hf	-3.81	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.831		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
tb	605.22	K	Joback Method
tc	846.26	K	Joback Method
tf	423.36	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.12	J/mol×K	605.22	Joback Method
cpg	272.72	J/mol×K	645.39	Joback Method

cpg	281.57	J/mol×K	685.57	Joback Method
cpg	289.71	J/mol×K	725.74	Joback Method
cpg	297.17	J/mol×K	765.91	Joback Method
cpg	303.98	J/mol×K	806.08	Joback Method
cpg	310.20	J/mol×K	846.26	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=C140385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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