

Urea, N'-(4-chlorophenyl)-N,N-dimethyl-

Other names:	1,1-Dimethyl-3-(p-chlorophenyl)thiourea 1,1-Dimethyl-3-(p-chlorophenyl)urea 1-(4-Chloro phenyl)-3,3-dimethyluree 1-(4-Chlorophenyl)-3,3-dimethylurea 1-(p-Chlorophenyl)-3,3-dimethylurea 3-(4-Chloor-fenyl)-1,1-dimethylureum 3-(4-Chlor-phenyl)-1,1-dimethyl-harnstoff 3-(4-Chlorophenyl)-1,1-dimethylurea 3-(4-cloro-fenil)-1,1-dimetil-urea 3-(p-Chlorophenyl)-1,1-dimethylurea 3-Methyl-4-oxo-2-phenyl-4h-1-benzopyran-8-carboxylic acid, 4-morpholinethyl ester, hydrochloride CMU Chlorfenidim Herbicides, monuron Karmex Monuron Herbicide Karmex W. monuron herbicide Lirobetarex Monurex Monuron Monurox Monuruon Monuuron N'-(4-Chlorophenyl)-N,N-dimethylurea N,N-Dimethyl-N'-(4-chlorophenyl)urea N-(4-Chlorophenyl)-N',N'-dimethylurea N-(p-Chlorophenyl)-N',N'-dimethylurea N-Dimethyl-N'-(4-chlorophenyl)urea NCI-C02846 NSC 8949 Telvar Telvar Monuron Weedkiller Telvar W. monuron weedkiller USAF P-8 USAF XR-41 Urea, 3-(p-chlorophenyl)-1,1-dimethyl-
Inchi:	InChI=1S/C9H11ClN2O/c1-12(2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
InchiKey:	BMLIZLVNXIYGCK-UHFFFAOYSA-N
Formula:	C9H11ClN2O
SMILES:	CN(C)C(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	198.65

Physical Properties

Property code	Value	Unit	Source
chs	-4861.80 ± 4.20	kJ/mol	NIST Webbook
gf	187.00	kJ/mol	Joback Method
hf	-11.35	kJ/mol	Joback Method
hfs	-272.00 ± 4.20	kJ/mol	NIST Webbook
hfus	26.63	kJ/mol	Joback Method
hsub	115.00	kJ/mol	NIST Webbook
hvap	58.18	kJ/mol	Joback Method
log10ws	-2.91		Aqueous Solubility Prediction Method
log10ws	-2.89		Estimated Solubility Method
logp	2.433		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	590.89	K	Joback Method
tc	811.66	K	Joback Method
tf	441.50 ± 0.20	K	NIST Webbook
tf	447.88 ± 0.20	K	NIST Webbook
tf	445.65	K	Aqueous Solubility Prediction Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.65	J/mol×K	590.89	Joback Method
cpg	350.07	J/mol×K	627.68	Joback Method
cpg	361.63	J/mol×K	664.48	Joback Method
cpg	372.36	J/mol×K	701.27	Joback Method
cpg	382.31	J/mol×K	738.07	Joback Method
cpg	391.52	J/mol×K	774.86	Joback Method
cpg	400.03	J/mol×K	811.66	Joback Method
hfust	29.30	kJ/mol	447.60	NIST Webbook
hfust	29.46	kJ/mol	447.60	NIST Webbook

hfust	29.46	kJ/mol	447.60	NIST Webbook
hsubt	114.60 ± 4.90	kJ/mol	341.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.86214e+01
Coeff. B	-1.37888e+04
Temperature range (K), min.	486.66
Temperature range (K), max.	591.54

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150685&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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