Diuron

Other names:

1,1-Dimethyl-3-(3,4-dichlorophenyl)urea
1-(3,4-Dichlorophenyl)-3,3-dimethylurea
3-(3,4-Dichloor-fenyl)-1,1-dimethylureum
3-(3,4-Dichlor-phenyl)-1,1-dimethyl-harnstoff
3-(3,4-Dichlorophenol)-1,1-dimethylurea
3-(3,4-Dichlorophenyl)-1,1-dimethylurea
3-(3,4-Dicloro-fenyl)-1,1-dimetil-urea
Aguron
Cekiuron
Crisuron
DCMU
DCMU 99
DMU
DP Hardener 95
Dailon
Di-On
Diater
Dichlorfenidim
Direx 4L
Direx 80W
Diuron 4L
Diuron Nortox
Duran
Dynex
HW 920
Herbatox
Karamex
Karmex
Karmex 80W
Karmex D
Karmex DL
Karmex DW
Karmex Diuron Herbicide
Lucenit
Marmer
N'-(3,4-Dichlorophenyl)-N,N-dimethylurea
N,N,-Dimethyl-N'-(3,4-dichlorophenyl)urea
N-(3,4-Dichlorophenyl)-N',N'-dimethylurea
Preventol A 6
Telvar Diuron Weed Killer

	Unidron
	Urea, 3-(3,4-dichlorophenyl)-1,1-dimethyl-
	Urea, N'-(3,4-dichlorophenyl)-N,N-dimethyl-
	Urox D
	Vonduron
	Xarmex
Inchi:	InChI=1S/C9H10Cl2N2O/c1-13(2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)
InchiKey:	XMTQQYYKAHVGBJ-UHFFFAOYSA-N
Formula:	C9H10Cl2N2O
SMILES:	CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	233.09
CAS:	330-54-1

Physical Properties

Property code	Value	Unit	Source
chs	-4681.90 ± 4.20	kJ/mol	NIST Webbook
gf	165.44	kJ/mol	Joback Method
hf	-38.56	kJ/mol	Joback Method
hfs	-329.00 ± 4.20	kJ/mol	NIST Webbook
hfus	30.44	kJ/mol	Joback Method
hsub	133.90 ± 0.70	kJ/mol	NIST Webbook
hvap	63.22	kJ/mol	Joback Method
log10ws	-1.22		Aqueous Solubility Prediction Method
log10ws	-3.80		Estimated Solubility Method
log10ws	-3.76		Aqueous and cosolvent solubility data for drug-like organic compounds
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	431.55	K	Aqueous Solubility Prediction Method
tf	430.70 ± 0.20	K	NIST Webbook
tf	429.70 ± 0.20	K	NIST Webbook
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
hfust	25.28	kJ/mol	435.10	NIST Webbook
hfust	30.47	kJ/mol	430.50	NIST Webbook
hfust	33.89	kJ/mol	429.70	NIST Webbook
hsubt	119.00 ± 0.60	kJ/mol	393.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C330541&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume