Metoxuron

Other names:	3-(3-Chlor-4-methoxyphenyl)-1,1-dimethylharnstoff
	3-(3-Chloro-4-methoxyphenyl)-1,1-dimethylurea
	Deftor
	Dosaflo
	Dosagran
	Dosanex
	Dosanex FL
	Dosanex MG
	FL
	Herbicide 6602
	Metoxuran
	N'-(3-Chlor-4-methoxy-phenyl)-N,N-dimethylharnstoff
	N'-(3-chloro-4-methoxyphenyl)-N,N-dimethylurea
	N,N-Dimethyl-N'-(4-methoxy-3-chlorophenyl)urea
	N-(3-Chloro-4-methoxyphenyl)-N',N'-dimethylurea
	Purivel
	SAN 6602
	SAN 6915H
	SAN 7102
	SAN 7102H
	Sulerex
	Urea, 3-(3-chloro-4-methoxyphenyl)-1,1-dimethyl-
	Urea, N'-(3-chloro-4-methoxyphenyl)-N,N-dimethyl-
Inchi:	InChI=1S/C10H13ClN2O2/c1-13(2)10(14)12-7-4-5-9(15-3)8(11)6-7/h4-6H,1-3H3,(H,12,1
InchiKey:	DSRNRYQBBJQVCW-UHFFFAOYSA-N
Formula:	C10H13ClN2O2
SMILES:	COc1ccc(NC(=O)N(C)C)cc1Cl
Mol. weight [g/mol]:	228.68
CAS:	19937-59-8

Physical Properties

Property code	Value	Unit	Source
gf	80.79	kJ/mol	Joback Method
hf	-175.68	kJ/mol	Joback Method
hfus	30.02	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method

log10ws	-2.56		Estimated Solubility Method
log10ws	-2.56		Aqueous Solubility Prediction Method
logp	2.442		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	641.17	K	Joback Method
tc	856.39	K	Joback Method
tf	399.82	K	Aqueous Solubility Prediction Method
tf	399.49 ± 0.20	K	NIST Webbook
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.51	J/mol×K	641.17	Joback Method
cpg	421.17	J/mol×K	677.04	Joback Method
cpg	433.02	J/mol×K	712.91	Joback Method
cpg	444.09	J/mol×K	748.78	Joback Method
cpg	454.39	J/mol×K	784.65	Joback Method
cpg	463.94	J/mol×K	820.52	Joback Method
cpg	472.78	J/mol×K	856.39	Joback Method
hfust	27.48	kJ/mol	399.20	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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19937598&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion 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

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