Monolinuron

Other names:	1-Methoxy-1-methyl-3-(4-chlorophenyl)urea
	3-(4-Chlorophenyl)-1-methoxy-1-methylurea
	3-(4-Chlorphenyl)-1-methoxy-1-methylharnstoff
	Afesin
	Aresin
	Arezin
	Arezine
	Arresin
	HOE 2747
	Monorotox
	N'-(4-Chlorophenyl)-N-methoxy-N-methylurea
	N-(4-Chlorophenyl)-N'-methoxy-N-methylurea
	Premalin
	Urea, 3-(p-chlorophenyl)-1-methoxy-1-methyl-
	Urea, N'-(4-chlorophenyl)-N-methoxy-N-methyl-
Inchi:	InChI=1S/C9H11ClN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
InchiKey:	LKJPSUCKSLORMF-UHFFFAOYSA-N
Formula:	C9H11ClN2O2
SMILES:	CON(C)C(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	214.65
CAS:	1746-81-2

Physical Properties

Property code	Value	Unit	Source
gf	82.00	kJ/mol	Joback Method
hf	-143.57	kJ/mol	Joback Method
hfus	27.82	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-2.57		Aqueous Solubility Prediction Method
log10ws	-2.57		Estimated Solubility Method
logp	2.365		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	613.31	K	Joback Method
tc	831.34	K	Joback Method

tf	354.65	K	Aqueous Solubility Prediction Method
tf	353.91 ± 0.20	K	NIST Webbook
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.14	J/mol×K	795.01	Joback Method
cpg	361.17	J/mol×K	613.31	Joback Method
cpg	373.34	J/mol×K	649.65	Joback Method
cpg	384.69	J/mol×K	685.99	Joback Method
cpg	395.26	J/mol×K	722.33	Joback Method
cpg	405.06	J/mol×K	758.67	Joback Method
cpg	422.50	J/mol×K	831.34	Joback Method
hfust	22.54	kJ/mol	353.40	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=C1746812&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