Chloroxuron

Other names:	1-(4-(4-Chloro-phenoxy)phenyl)-3,3-d'methyluree
	3-(4-(4-Chloor-fenoxy)-fenyl)-1,1-dimethylureum
	3-(4-(4-Chlor-phenoxy)-phenyl)-1,1-dimethylharnstoff
	3-(4-(4-Chloro-fenossil)fenil)-1,1-dimetil-urea
	3-(p-(p-Chlorophenoxy)phenyl)-1,1-dimethylurea
	3-[4-(4-Chlorophenoxy)phenyl]-1,1-dimethylurea
	C 1983
	CIBA 1983
	Chloroxifenidim
	Chloroxyfenidim
	Chlorphencarb
	Gesamoos
	N'-4-(p-Chlorophenoxy)phenyl-N,N-dimethylurea
	N'-[4-(4-Chlorophenoxy)phenyl]-N,N-dimethylurea
	Norex
	Tenoran
	Urea, 3-[p-(p-chlorophenoxy)phenyl]-1,1-dimethyl-
	Urea, N'-[4-(4-chlorophenoxy)phenyl]-N,N-dimethyl-
Inchi:	InChI=1S/C15H15ClN2O2/c1-18(2)15(19)17-12-5-9-14(10-6-12)20-13-7-3-11(16)4-8-13/h
InchiKey:	IVUXTESCPZUGJC-UHFFFAOYSA-N
Formula:	C15H15ClN2O2
SMILES:	CN(C)C(=O)Nc1ccc(Oc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	290.75
CAS:	1982-47-4

Physical Properties

Property code	Value	Unit	Source
gf	235.30	kJ/mol	Joback Method
hf	-42.35	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	76.88	kJ/mol	Joback Method
log10ws	-4.89		Aqueous Solubility Prediction Method
log10ws	-4.89		Estimated Solubility Method
logp	4.226		Crippen Method
mcvol	214.330	ml/mol	McGowan Method

pc	2485.07	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	782.25	K	Joback Method
tc	1017.90	K	Joback Method
tf	425.83 ± 0.20	K	NIST Webbook
tf	425.10 ± 0.20	K	NIST Webbook
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.20	J/mol×K	978.62	Joback Method
cpg	580.26	J/mol×K	782.25	Joback Method
cpg	593.64	J/mol×K	821.52	Joback Method
cpg	605.86	J/mol×K	860.80	Joback Method
cpg	616.99	J/mol×K	900.07	Joback Method
cpg	627.09	J/mol×K	939.35	Joback Method
cpg	644.39	J/mol×K	1017.90	Joback Method
hfust	34.87	kJ/mol	425.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C1982474&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume