Urea, N'-[4-(4-chlorophenoxy)phenyl]-N,N-dimethyl-

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-
chloroxuron

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

Physical Properties

Property code	Value	Unit	Source
hfus	37.01	kJ/mol	Joback Method
ie	7.36	eV	Cheméo Relay (1.0)
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
tf	443.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	636.20	J/mol×K	978.62	Joback Method
cpg	644.39	J/mol×K	1017.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1982474&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Octanol/Water Partition Coefficient of Selected Herbicides: Determination Using Shake-Flask Method and Reversed-Phase High-Performance Liquid Chromatography:	https://www.doi.org/10.1021/je049947x
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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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