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

Other names: C 3470
Difenoxuron
Difenoxurone
Lironion
N'-(4-(4-Methoxyphenoxy)phenyl)-N,N-dimethylurea
Pinoran
Urea, 1,1-dimethyl-3-(p-(p-methoxyphenoxy)phenyl)-

Inchi: InChI=1S/C16H18N2O3/c1-18(2)16(19)17-12-4-6-14(7-5-12)21-15-10-8-13(20-3)9-11-15

InchiKey: AMVYOVYGIJXTQB-UHFFFAOYSA-N

Formula: C16H18N2O3

SMILES: COc1ccc(Oc2ccc(NC(=O)N(C)C)cc2)cc1

Mol. weight [g/mol]: 286.33

CAS: 14214-32-5

Physical Properties

Property code	Value	Unit	Source
gf	150.65	kJ/mol	Joback Method
hf	-179.47	kJ/mol	Joback Method
hfus	36.59	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-4.16		Aqueous Solubility Prediction Method
log10ws	-4.16		Estimated Solubility Method
logp	3.581		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
tb	790.12	K	Joback Method
tc	1016.83	K	Joback Method
tf	527.48	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	636.97	J/mol×K	790.12	Joback Method
cpg	651.44	J/mol×K	827.90	Joback Method
cpg	664.70	J/mol×K	865.69	Joback Method
cpg	676.79	J/mol×K	903.47	Joback Method
cpg	687.74	J/mol×K	941.26	Joback Method
cpg	697.59	J/mol×K	979.04	Joback Method
cpg	706.37	J/mol×K	1016.83	Joback Method

Sources

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=C14214325&Units=SI

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

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
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