Difluron

Other names:	1-(4-Chlorophenyl)-3-(2,6-difluorobenzoyl)urea
	AI3-29054
	Benzamide, N-[[(4-chlorophenyl)amino]carbonyl]-2,6-difluoro-
	DU 112307
	Diflubenzuron
	Dimilin
	Duphacid
	ENT-29054
	Larvakil
	Micromite
	N-[(4-chlorophenyl)carbamoyl]-2,6-difluorobenzamide
	N-[[(4-Chlorophenyl)amno]carbonyl]-2,6-difluorobenzamide
	N-[[(4-chlorophenyl)amino]carbonyl]-2,6-difluorobenzamide
	OMS 1804
	PDD 6040-I
	PH 60-40
	TH 6040
	Thompson-Hayward 6040
Inchi:	InChI=1S/C14H9ClF2N2O2/c15-8-4-6-9(7-5-8)18-14(21)19-13(20)12-10(16)2-1-3-11(12)
InchiKey:	QQQYTWIFVNKMRW-UHFFFAOYSA-N
Formula:	C14H9ClF2N2O2
SMILES:	O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	310.68
CAS:	35367-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-217.68	kJ/mol	Joback Method
hf	-419.82	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-6.02		Estimated Solubility Method
log10ws	-6.21		Aqueous Solubility Prediction Method
logp	3.580		Crippen Method
mcvol	199.480	ml/mol	McGowan Method

pc	2712.67	kPa	Joback Method
tb	832.07	K	Joback Method
tc	1063.69	K	Joback Method
tf	501.18 ± 0.20	K	NIST Webbook
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.30	J/mol×K	832.07	Joback Method
cpg	543.90	J/mol×K	870.67	Joback Method
cpg	552.57	J/mol×K	909.28	Joback Method
cpg	560.39	J/mol×K	947.88	Joback Method
cpg	567.39	J/mol×K	986.48	Joback Method
cpg	573.64	J/mol×K	1025.09	Joback Method
cpg	579.18	J/mol×K	1063.69	Joback Method
hfust	55.99	kJ/mol	499.50	NIST Webbook

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=C35367385&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
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