TEFLUBENZURON

Other names: N-[(3,5-dichloro-2,4-difluorophenyl)carbamoyl]-2,6-difluorobenzamide
Inchi: InChI=1S/C14H6Cl2F4N2O2/c15-5-4-8(12(20)10(16)11(5)19)21-14(24)22-13(23)9-6(17)
InchiKey: CJDWRQLODFKPEL-UHFFFAOYSA-N
Formula: C14H6Cl2F4N2O2
SMILES: O=C(NC(=O)c1c(F)cccc1F)Nc1cc(Cl)c(F)c(Cl)c1F
Mol. weight [g/mol]: 381.11

Physical Properties

Property code	Value	Unit	Source
gf	-648.12	kJ/mol	Joback Method
hf	-862.19	kJ/mol	Joback Method
hfus	51.87	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-7.42		Aqueous Solubility Prediction Method
log10ws	-7.28		Estimated Solubility Method
logp	4.512		Crippen Method
mcvol	215.260	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
tb	882.98	K	Joback Method
tc	1105.65	K	Joback Method
tf	495.65	K	Aqueous Solubility Prediction Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.77	J/mol×K	882.98	Joback Method
cpg	569.32	J/mol×K	920.09	Joback Method
cpg	576.09	J/mol×K	957.20	Joback Method
cpg	582.10	J/mol×K	994.31	Joback Method
cpg	587.37	J/mol×K	1031.43	Joback Method
cpg	591.95	J/mol×K	1068.54	Joback Method

cpg	595.86	J/mol×K	1105.65	Joback Method

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
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
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