

Dimefuron

Other names: 3-[4-(5-tert-butyl-2-oxo-1,3,4-oxadiazol-3-yl)-3-chlorophenyl]-1,1-dimethylurea
Inchi: InChI=1S/C15H19ClN4O3/c1-15(2,3)12-18-20(14(22)23-12)11-7-6-9(8-10(11)16)17-13(2)
InchiKey: DHWRNDJOGMTCPB-UHFFFAOYSA-N
Formula: C15H19ClN4O3
SMILES: CN(C)C(=O)Nc1ccc(-n2nc(C(C)(C)C)oc2=O)c(Cl)c1
Mol. weight [g/mol]: 338.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Aqueous Solubility Prediction Method
log10ws	-4.33		Estimated Solubility Method
logp	2.870		Crippen Method
mcvol	244.460	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/101-118-8/Dimefuron.pdf>

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