

Chlorimuron-ethyl (ph 7)

Other names:	ethyl 2-[[[(4-chloro-6-methoxypyrimidin-2-yl)-formylamino]sulfamoyl]benzoate
Inchi:	InChI=1S/C15H15ClN4O6S/c1-3-26-14(22)10-6-4-5-7-11(10)27(23,24)19-20(9-21)15-17
InchiKey:	MBDMKWJEKDHRRP-UHFFFAOYSA-N
Formula:	C15H15ClN4O6S
SMILES:	CCOC(=O)c1cccc1S(=O)(=O)NN(C=O)c1nc(Cl)cc(OC)n1
Mol. weight [g/mol]:	414.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Aqueous Solubility Prediction Method
log10ws	-4.58		Estimated Solubility Method
logp	1.172		Crippen Method
mcvol	269.820	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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/105-844-8/Chlorimuron-ethyl-ph-7.pdf>

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