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)c1ccccc1S(=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/ci990307l
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