

3-chloro-6-diethoxyphosphinothioxyloxy-4-methylchromen-2-one

Inchi: InChI=1S/C14H16ClO5PS/c1-4-17-21(22,18-5-2)20-10-6-7-12-11(8-10)9(3)13(15)14(16)
InchiKey: SJNIEBAPMPPLYAB-UHFFFAOYSA-N
Formula: C14H16ClO5PS
SMILES: CCOP(=S)(OCC)Oc1ccc2oc(=O)c(Cl)c(C)c2c1
Mol. weight [g/mol]: 362.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Aqueous Solubility Prediction Method
logp	4.431		Crippen Method
mcvol	243.300	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

Legend

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

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