2-[4-(diethoxyphosphorylmethyl)phenyl]-1,3-benz

Inchi: InChI=1S/C18H20NO3PS/c1-3-21-23(20,22-4-2)13-14-9-11-15(12-10-14)18-19-16-7-5-6
InchiKey: FVYRUSCZCWSFLT-UHFFFAOYSA-N
Formula: C18H20NO3PS
SMILES: CCOP(=O)(Cc1ccc(-c2nc3ccccc3s2)cc1)OCC
Mol. weight [g/mol]: 361.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Aqueous Solubility Prediction Method
logp	5.729		Crippen Method
mcvol	266.200	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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