1-[[4-(1,3-benzothiazol-2-yl)phenyl]methyl-ethoxy

Inchi: InChI=1S/C20H21N2O3PS/c1-2-25-26(24,22-13-5-8-19(22)23)14-15-9-11-16(12-10-15)2

InchiKey: HTAUUADKDLLMRU-UHFFFAOYSA-N

Formula: C20H21N2O3PS

SMILES: CCOP(=O)(Cc1ccc(-c2nc3ccccc3s2)cc1)N1CCCC1=O

Mol. weight [g/mol]: 400.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Aqueous Solubility Prediction Method
logp	5.315		Crippen Method
mcvol	289.200	ml/mol	McGowan Method

Sources

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume