meloxicam

Inchi: InChI=1S/C14H13N3O4S2/c1-8-7-15-14(22-8)16-13(19)11-12(18)9-5-3-4-6-10(9)23(20,2

InchiKey: ZRVUJXDFFKFLMG-UHFFFAOYSA-N

Formula: C14H13N3O4S2

SMILES: Cc1cnc(NC(=O)C2=C(O)c3ccccc3S(=O)(=O)N2C)s1

Mol. weight [g/mol]: 351.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Aqueous Solubility Prediction Method
logp	1.951		Crippen Method
mcvol	231.560	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