Mebendazole

Inchi: InChI=1S/C16H13N3O3/c1-22-16(21)19-15-17-12-8-7-11(9-13(12)18-15)14(20)10-5-3-2-
InchiKey: OPXLLQIJSORQAM-UHFFFAOYSA-N
Formula: C16H13N3O3
SMILES: COC(=O)Nc1nc2ccc(C(=O)c3ccccc3)cc2[nH]1
Mol. weight [g/mol]: 295.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Aqueous Solubility Prediction Method
log10ws	-3.88		Estimated Solubility Method
logp	2.490		Crippen Method
mcvol	212.570	ml/mol	McGowan Method
tf	561.65	K	Aqueous Solubility Prediction 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
tf: Normal melting (fusion) point

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