SCHEMBL9488362

Inchi: InChI=1S/C18H21NO3/c1-19-8-7-18-10-12(20)4-5-13(18)14(19)9-11-3-6-15(22-2)17(21)
InchiKey: SLJDAVMWFVYEFI-UHFFFAOYSA-N
Formula: C18H21NO3
SMILES: COc1ccc2c(c1O)C13CCN(C)C(C2)C1C=CC(=O)C3
Mol. weight [g/mol]: 299.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Aqueous Solubility Prediction Method
logp	2.044		Crippen Method
mcvol	227.130	ml/mol	McGowan Method
tf	424.65	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
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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