Khellin

Inchi: InChI=1S/C14H12O5/c1-7-6-9(15)10-11(16-2)8-4-5-18-12(8)14(17-3)13(10)19-7/h4-6H,1
InchiKey: HSMPDPBYAYSOBC-UHFFFAOYSA-N
Formula: C14H12O5
SMILES: COc1c2occc2c(OC)c2c(=O)cc(C)oc12
Mol. weight [g/mol]: 260.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Aqueous Solubility Prediction Method
log10ws	-3.02		Estimated Solubility Method
logp	2.865		Crippen Method
mcvol	179.090	ml/mol	McGowan Method

Sources

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
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.