Furomollugin

Inchi: InChI=1S/C14H10O4/c1-17-14(16)11-10-6-7-18-13(10)9-5-3-2-4-8(9)12(11)15/h2-7,15H,
InchiKey: AFMYCYWCHKTNNE-UHFFFAOYSA-N
Formula: C14H10O4
SMILES: COC(=O)c1c(O)c2ccccc2c2occc12
Mol. weight [g/mol]: 242.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	3.078		Crippen Method
mcvol	168.920	ml/mol	McGowan Method
rinpol	2080.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R513710&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices