4,9-dimethoxypsoralen

Inchi: InChI=1S/C13H10O5/c1-15-9-6-10(14)18-12-8(9)5-7-3-4-17-11(7)13(12)16-2/h3-6H,1-2H
InchiKey: KAWXJSCFXZDZAR-UHFFFAOYSA-N
Formula: C13H10O5
SMILES: COc1cc(=O)oc2c(OC)c3occc3cc12
Mol. weight [g/mol]: 246.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.21		Crippen Method
logp	2.556		Crippen Method
mcvol	165.000	ml/mol	McGowan Method
rinpol	2031.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R219339&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpol: Non-polar retention indices