4-methoxypsoralen

Inchi: InChI=1S/C12H8O4/c1-14-10-6-12(13)16-11-5-9-7(2-3-15-9)4-8(10)11/h2-6H,1H3
InchiKey: IFBJMRYEEKIECT-UHFFFAOYSA-N
Formula: C12H8O4
SMILES: COc1cc(=O)oc2cc3occc3cc12
Mol. weight [g/mol]: 216.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.09		Crippen Method
logp	2.548		Crippen Method
mcvol	145.040	ml/mol	McGowan Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R219344&Units=SI
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
rinpol: Non-polar retention indices

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