2-Isopropylpsoralen

Inchi: InChI=1S/C14H12O3/c1-8(2)11-6-10-5-9-3-4-14(15)17-12(9)7-13(10)16-11/h3-8H,1-2H3
InchiKey: KVHBNBMOEQQULB-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: CC(C)c1cc2cc3ccc(=O)oc3cc2o1
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.16		Crippen Method
logp	3.663		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R423924&Units=SI

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.