Auraptenol

Inchi: InChI=1S/C15H16O4/c1-9(2)12(16)8-11-13(18-3)6-4-10-5-7-14(17)19-15(10)11/h4-7,12,
InchiKey: SQSRYWNOKPJENY-UHFFFAOYSA-N
Formula: C15H16O4
SMILES: C=C(C)C(O)Cc1c(OC)ccc2ccc(=O)oc12
Mol. weight [g/mol]: 260.29
CAS: 51559-35-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.84		Crippen Method
logp	2.281		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	2298.40		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=C51559354&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.