

bromadiolone

Inchi: InChI=1S/C30H23BrO4/c31-23-16-14-20(15-17-23)19-10-12-22(13-11-19)26(32)18-25(2
InchiKey: OWNRRUFOJXFKCU-UHFFFAOYSA-N
Formula: C30H23BrO4
SMILES: O=c1oc2ccccc2c(O)c1C(CC(O)c1ccc(-c2ccc(Br)cc2)cc1)c1ccccc1
Mol. weight [g/mol]: 527.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Aqueous Solubility Prediction Method
log10ws	-4.45		Estimated Solubility Method
logp	7.184		Crippen Method
mvol	360.040	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mvol: McGowan's characteristic volume

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<https://www.cheméo.com/cid/106-396-5/bromadiolone.pdf>

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