

diphenhydramine

Inchi: InChI=1S/C14H12FNO3/c1-7-2-3-8-4-9(15)5-10-12(8)16(7)6-11(13(10)17)14(18)19/h4-7
InchiKey: DPSPPJIUMHPXMA-UHFFFAOYSA-N
Formula: C14H12FNO3
SMILES: CC1CCc2cc(F)cc3c(=O)c(C(=O)O)cn1c23
Mol. weight [g/mol]: 261.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Aqueous Solubility Prediction Method
logp	2.346		Crippen Method
mcvol	179.100	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/AqueousDataset002.xlsx>
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

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<https://www.cheméo.com/cid/108-436-8/diphenhydramine.pdf>

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