

ethyl eburnamenine-14-carboxylate

Inchi: InChI=1S/C22H26N2O2/c1-3-22-11-7-12-23-13-10-16-15-8-5-6-9-17(15)24(19(16)20(22)
InchiKey: DDNCQMVWWZOMLN-UHFFFAOYSA-N
Formula: C22H26N2O2
SMILES: CCOC(=O)C1=CC2(CC)CCCN3CCc4c(n1c1cccc41)C32
Mol. weight [g/mol]: 350.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Aqueous Solubility Prediction Method
logp	4.148		Crippen Method
mcvol	272.440	ml/mol	McGowan Method

Sources

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>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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