

norbormide

Inchi: InChI=1S/C33H25N3O3/c37-31-28-22-19-23(33(39,21-13-5-2-6-14-21)25-16-8-10-18-35
InchiKey: DNTHHIVFNQZZRD-UHFFFAOYSA-N
Formula: C33H25N3O3
SMILES: O=C1NC(=O)C2C3C(C(O)(c4ccccc4)c4ccccc4)=CC(C3=C(c3ccccc3)c3ccccc3)C12
Mol. weight [g/mol]: 511.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Aqueous Solubility Prediction Method
log10ws	-3.93		Estimated Solubility Method
logp	4.289		Crippen Method
mcvol	378.560	ml/mol	McGowan Method

Sources

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>
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>

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/101-147-6/norbormide.pdf>

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