

Clofazimine

Inchi: InChI=1S/C27H22Cl2N4/c1-17(2)30-24-16-27-25(15-23(24)31-20-11-7-18(28)8-12-20)32
InchiKey: WDQPAMHFFCXSNU-UHFFFAOYSA-N
Formula: C27H22Cl2N4
SMILES: CC(C)N=c1cc2n(-c3ccc(Cl)cc3)c3ccccc3nc-2cc1Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 473.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Aqueous Solubility Prediction Method
log10ws	-5.80		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	7.490		Crippen Method
mccvol	345.490	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
Aqueous and cosolvent solubility data for drug-like organic compounds: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/112-573-1/Clofazimine.pdf>

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