

nevirapine

Other names: 129618-40-2
Inchi: InChI=1S/C15H14N4O/c1-9-6-8-17-14-12(9)18-15(20)11-3-2-7-16-13(11)19(14)10-4-5-1
InchiKey: NQDJXKOVJZTUJA-UHFFFAOYSA-N
Formula: C15H14N4O
SMILES: Cc1ccnc2c1NC(=O)c1cccnc1N2C1CC1
Mol. weight [g/mol]: 266.30

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -3.19 | | Aqueous Solubility Prediction Method |
| log10ws | -3.19 | | Estimated Solubility Method |
| logp | 2.651 | | Crippen Method |
| mcvol | 194.460 | ml/mol | McGowan Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

Legend

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

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