

perlapine

Inchi: InChI=1S/C19H21N3/c1-21-10-12-22(13-11-21)19-17-8-4-2-6-15(17)14-16-7-3-5-9-18(16)
InchiKey: PWRPUAKXMQAFCJ-UHFFFAOYSA-N
Formula: C19H21N3
SMILES: CN1CCN(C2=Nc3ccccc3Cc3ccccc32)CC1
Mol. weight [g/mol]: 291.39
CAS: 1977-11-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.31 | | Crippen Method |
| logp | 2.917 | | Crippen Method |
| mcvol | 234.970 | ml/mol | McGowan Method |
| rinpola | 2421.00 | | NIST Webbook |
| rinpola | 2421.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1977113&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/28-147-8/perlapine.pdf>

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