

7-Hydroxyamoxapine

Inchi: InChI=1S/C17H16ClN3O2/c18-11-1-4-15-13(9-11)17(21-7-5-19-6-8-21)20-14-3-2-12(22)
InchiKey: MEUGUMOVYNSGEW-UHFFFAOYSA-N
Formula: C17H16ClN3O2
SMILES: Oc1ccc2c(c1)Oc1ccc(Cl)cc1C(N1CCNCC1)=N2
Mol. weight [g/mol]: 329.78
CAS: 37081-76-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.27 | | Crippen Method |
| logp | 3.135 | | Crippen Method |
| mcvol | 230.770 | ml/mol | McGowan Method |
| rinpol | 2900.00 | | NIST Webbook |
| rinpol | 2900.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C37081768&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/49-545-3/7-Hydroxyamoxapine.pdf>

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