

Chavicine

Inchi: InChI=1S/C17H19NO3/c19-17(18-10-4-1-5-11-18)7-3-2-6-14-8-9-15-16(12-14)21-13-20-
InchiKey: MXXWOMGUGJBKIW-PORYWJCVSA-N
Formula: C17H19NO3
SMILES: O=C(C=CC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 285.34
CAS: 495-91-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.95 | | Crippen Method |
| logp | 2.997 | | Crippen Method |
| mcvol | 219.600 | ml/mol | McGowan Method |
| rinpola | 2649.60 | | NIST Webbook |
| rinpola | 2649.60 | | NIST Webbook |

Sources

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=C495910&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/122-551-4/Chavicine.pdf>

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