

Haloxazolam

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|-----------------------------|---|
| Other names: | Oxazolo[3,2-d](1,4)benzodiazepin-6(5H)-one, 2,3,7,11b-tetrahydro-10-bromo-11b-(2-fluorophenyl)- 10-Bromo-11b-(2-fluorophenyl)-2,3,7,11b-tetrahydrooxazolo[3,2-d](1,4)benzodiazepin-6(5H) CS-430 Somelin 10-Bromo-11b-(o-fluorophenyl)-2,3,7,11b-tetrahydrooxazolo[3,2-d][1,4]benzodiazepin-6(5H) |
| Inchi: | InChI=1S/C17H14BrFN2O2/c18-11-5-6-15-13(9-11)17(12-3-1-2-4-14(12)19)21(7-8-23-17) |
| InchiKey: | XDKCGKQHVB00HC-UHFFFAOYSA-N |
| Formula: | C17H14BrFN2O2 |
| SMILES: | OC1=Nc2ccc(Br)cc2C2(c3ccccc3F)OCCN2C1 |
| Mol. weight [g/mol]: | 377.21 |
| CAS: | 59128-97-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.40 | | Crippen Method |
| logp | 3.723 | | Crippen Method |
| mcvol | 227.820 | ml/mol | McGowan Method |
| rinpol | 2620.00 | | NIST Webbook |
| rinpol | 2646.00 | | NIST Webbook |
| rinpol | 2620.00 | | NIST Webbook |
| rinpol | 2634.00 | | NIST Webbook |
| rinpol | 2634.00 | | NIST Webbook |
| rinpol | 2620.00 | | NIST Webbook |
| rinpol | 2646.00 | | 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=C59128971&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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