# Loxapine

| | |
|---|---|
| **Other names:** | 2-Chloro-11-(4-methyl-1-piperazinyl)dibenz[b,f][1,4]oxazepine |
| | 2-Chloro-11-(4-methylpiperazino)dibenz[b,f][1,4]oxazepine |
| | 8-chloro-6-(4-methylpiperazin-1-yl)benzo[b][1,5]benzoxazepine |
| | CL-62362 |
| | CL-71563 |
| | Cloxazepine |
| | Dibenz[b,f][1,4]oxazepine, 2-chloro-11-(4-methyl-1-piperazinyl)- |
| | Dibenzacepin |
| | Dibenzoazepine |
| | HF3170 |
| | LW 3170 |
| | Loxapin |
| | Loxepine |
| | Loxitane |
| | Loxitane IM |
| | Oxilapine |
| | S-805 |
| | SUM 3170 |
| **Inchi:** | InChI=1S/C18H18ClN3O/c1-21-8-10-22(11-9-21)18-14-12-13(19)6-7-16(14)23-17-5-3-2- |
| **InchiKey:** | XJGVXQDUIWGIRW-UHFFFAOYSA-N |
| **Formula:** | C18H18ClN3O |
| **SMILES:** | CN1CCN(C2=Nc3ccccc3Oc3ccc(Cl)cc32)CC1 |
| **Mol. weight [g/mol]:** | 327.81 |
| **CAS:** | 1977-10-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.42 | | Aqueous Solubility Prediction Method |
| logp | 3.771 | | Crippen Method |
| mcvol | 238.990 | ml/mol | McGowan Method |
| rinpol | 2542.00 | | NIST Webbook |
| rinpol | 2542.00 | | NIST Webbook |
| rinpol | 2530.00 | | NIST Webbook |
| rinpol | 2542.00 | | NIST Webbook |
| tf | 382.65 | K | Aqueous Solubility Prediction Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1977102&Units=SI |
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tf:** | Normal melting (fusion) point |

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