

Opipramol

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| Other names: | 1-Piperazineethanol, 4-[3-(5H-dibenz[b,f]azepin-5-yl)propyl]- Endison G 33040 GR 33040 N-[3-[4-(2-Hydroxyethyl)-piperazino]propyl]iminostilbene Nisidana Opipramol G Opramidol Insidon (free base) Insidon, base Pramolan (free base) 4-(3-(5H-Dibenz(b,f)azepin-5-yl)propyl)-1-piperazineethanol 5H-Dibenz(b,f)azepine, 5-(3-(4-(2-hydroxyethyl)-1-piperazinyl)propyl)- NSC 169867 |
| Inchi: | InChI=1S/C23H29N3O/c27-19-18-25-16-14-24(15-17-25)12-5-13-26-22-8-3-1-6-20(22)1 |
| InchiKey: | YNZFUWZUGRBMHL-UHFFFAOYSA-N |
| Formula: | C23H29N3O |
| SMILES: | OCCN1CCN(CCCN2c3ccccc3C=Cc3ccccc32)CC1 |
| Mol. weight [g/mol]: | 363.50 |
| CAS: | 315-72-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.67 | | Crippen Method |
| logp | 3.309 | | Crippen Method |
| mcvol | 297.200 | ml/mol | McGowan Method |

Sources

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|------------------------|---|
| 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=C315720&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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