

Methoxypromazine

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|-----------------------------|---|
| Other names: | 10H-Phenothiazine-10-propanamine, 2-methoxy-N,N-dimethyl-Phenothiazine, 10-[3-(dimethylamino)propyl]-2-methoxy-Methopromazine Tenton Tentone 10-[3-(Dimethylamino)propyl]-2-methoxyphenothiazine 2-Methoxy-10-[3'-(dimethylamino)propyl]phenothiazine 2-Methoxypromazine 4632 R.P Neoproma RP 4632 2-Methoxy-N,N-dimethyl-10H-phenothiazine-10-propanamine |
| Inchi: | InChI=1S/C18H22N2OS/c1-19(2)11-6-12-20-15-7-4-5-8-17(15)22-18-10-9-14(21-3)13-16 |
| InchiKey: | BRABPYPSZVCCLR-UHFFFAOYSA-N |
| Formula: | C18H22N2OS |
| SMILES: | COc1ccc2c(c1)N(CCCN(C)C)c1ccccc1S2 |
| Mol. weight [g/mol]: | 314.44 |
| CAS: | 61-01-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.20 | | Crippen Method |
| logp | 4.250 | | Crippen Method |
| mcvol | 248.280 | ml/mol | McGowan Method |
| rinpol | 2542.00 | | NIST Webbook |
| rinpol | 2542.00 | | 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=C61018&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 |
| rinpol: | Non-polar retention indices |

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