

Metixene

Other names:

Piperidine, 1-methyl-3-(9H-thioxanthen-9-ylmethyl)-
Piperidine, 1-methyl-3-(thioxanthen-9-ylmethyl)-
Methixen
1-Methyl-3-(thioxanthen-9-ylmethyl) piperidine
Methixene
1-Methyl-3-(9H-thioxanthen-9-ylmethyl)piperidine
60 SJ 1977
Tremaril
Tremonil
Trest

Inchi: InChI=1S/C20H23NS/c1-21-12-6-7-15(14-21)13-18-16-8-2-4-10-19(16)22-20-11-5-3-9-1**InchiKey:** MJFJKKXQDNNUJF-UHFFFAOYSA-N**Formula:** C20H23NS**SMILES:** CN1CCCC(CC2c3ccccc3Sc3ccccc32)C1**Mol. weight [g/mol]:** 309.47**CAS:** 4969-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	5.015		Crippen Method
mcvol	249.750	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
rinpol	2470.00		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=C4969022&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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