

Trimeprazine

Other names:	Alimemazine 10H-Phenothiazine-10-propanamine, N,N,«beta»-trimethyl- Phenothiazine, 10-[3-(dimethylamino)-2-methylpropyl]- Alimezine Bayer 1219 Methylpromazine Repetin Teralen Teralene 10-[2-Methyl-3-(dimethylamino)propyl]phenothiazine 10-[3-(Dimethylamino)-2-methylpropyl]phenothiazine Trimeperazine (. +/-.)-Alimemazine (. +/-.)-Trimeprazine dl-Trimeprazine
Inchi:	InChI=1S/C18H22N2S/c1-14(12-19(2)3)13-20-15-8-4-6-10-17(15)21-18-11-7-5-9-16(18)
InchiKey:	ZZHLYYDVIOPZBE-UHFFFAOYSA-N
Formula:	C18H22N2S
SMILES:	CC(CN(C)C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	298.45
CAS:	84-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	4.487		Crippen Method
mcvol	242.410	ml/mol	McGowan Method
rinpol	2283.00		NIST Webbook
rinpol	2354.00		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=C84968&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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