

Methdilazine

Other names:	10H-Phenothiazine, 10-[(1-methyl-3-pyrrolidiny)methyl]- Phenothiazine, 10-[(1-methyl-3-pyrrolidiny)methyl]- MJ 5022 Tacaryl 10-[(1-Methyl-3-Pyrrolidiny)methyl]phenothiazine NCI-C60720 Tacazyl Product 5022 Tacryl
Inchi:	InChI=1S/C18H20N2S/c1-19-11-10-14(12-19)13-20-15-6-2-4-8-17(15)21-18-9-5-3-7-16(
InchiKey:	HTMIBDQKFHUPSX-UHFFFAOYSA-N
Formula:	C18H20N2S
SMILES:	CN1CCC(CN2c3ccccc3Sc3ccccc32)C1
Mol. weight [g/mol]:	296.43
CAS:	1982-37-2

Physical Properties

Property code	Value	Unit	Source
ie	7.25 ± 0.10	eV	NIST Webbook
log10ws	-4.15		Crippen Method
logp	4.241		Crippen Method
mcvol	231.550	ml/mol	McGowan Method
rinpol	2421.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2421.00		NIST Webbook
rinpol	2467.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1982372&Units=SI

Legend

ie:	Ionization energy
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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