

10H-Phenothiazine-10-propanamine, 2-methoxy-N,N,«beta»-trimethyl-

Other names:	Phenothiazine, 10-[3-(dimethylamino)-2-methylpropyl]-2-methoxy-10-(3-(Dimethylamino)-2-methylpropyl)-2-methoxyphenothiazine (.+/-.)-Methotrimeprazine dl-Methotrimeprazine 2-Methoxy-N,N,«beta»-trimethyl-10H-phenothiazine-10-propylamine 2-Methoxy-N,N,beta-trimethyl-10H-phenothiazine-10-propylamine Methotrimeprazine Levomepromazine Levomepropazine
Inchi:	InChI=1S/C19H24N2OS/c1-14(12-20(2)3)13-21-16-7-5-6-8-18(16)23-19-10-9-15(22-4)11
InchiKey:	VRQVVMDWGGWHTJ-UHFFFAOYSA-N
Formula:	C19H24N2OS
SMILES:	COc1ccc2c(c1)N(CC(C)CN(C)C)c1ccccc1S2
Mol. weight [g/mol]:	328.47
CAS:	851-68-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	4.496		Crippen Method
mcvol	262.370	ml/mol	McGowan Method
rinpol	2510.00		NIST Webbook
rinpol	2557.00		NIST Webbook
rinpol	2532.00		NIST Webbook
rinpol	2512.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2536.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2538.00		NIST Webbook
rinpol	2539.00		NIST Webbook
rinpol	2540.00		NIST Webbook
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rinpol	2540.00		NIST Webbook
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rinpol	2543.00	NIST Webbook
rinpol	2563.00	NIST Webbook
rinpol	2542.00	NIST Webbook
rinpol	2540.00	NIST Webbook
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rinpol	2538.00	NIST Webbook
rinpol	2540.00	NIST Webbook
rinpol	2545.00	NIST Webbook
rinpol	2530.00	NIST Webbook
rinpol	2535.00	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=C851683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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