

Dimetindene

Other names:	1H-Indene-2-ethanamine, N,N-dimethyl-3-[1-(2-pyridinyl)ethyl]- Pyridine, 2-(1-(2-(2-(dimethylamino)ethyl)inden-3-yl)ethyl)- Dimethindene Dimethpyrindene 2-(1-(2-(2-Dimethylaminoethyl)inden-3-yl)ethyl)pyridine Forhista 3614-69-5 (maleate) demethindene
Inchi:	InChI=1S/C20H24N2/c1-15(19-10-6-7-12-21-19)20-17(11-13-22(2)3)14-16-8-4-5-9-18(16)
InchiKey:	MVMQESMQSYOVGV-UHFFFAOYSA-N
Formula:	C20H24N2
SMILES:	CC(C1=C(CCN(C)C)Cc2ccccc21)c1cccn1
Mol. weight [g/mol]:	292.42
CAS:	5636-83-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	4.147		Crippen Method
mcpol	249.940	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2270.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5636839&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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