

Dimetacrine

Other names:	Acridan, 10-(3-(dimethylamino)propyl)-9,9-dimethyl- Dimetacrino Dimetacrinum Dimethacrin Dimethacrine N,N,9,9-Tetramethyl-10(9H)-acridinepropanamine 10(9H)-Acridinepropanamine, N,N,9,9-tetramethyl- 10-(3-(Dimethylamino)propyl)-9,9-dimethylacridan Acridan, 9,9-dimethyl-10-(3-(dimethylamino)propyl)- Dimethacin Dimethacine 9,9-Dimethyl-10-(3-(dimethylamino)propyl)acridan NSC 100297
Inchi:	InChI=1S/C20H26N2/c1-20(2)16-10-5-7-12-18(16)22(15-9-14-21(3)4)19-13-8-6-11-17(19)
InchiKey:	RYQOGSFEJBUZBX-UHFFFAOYSA-N
Formula:	C20H26N2
SMILES:	CN(C)CCCN1c2ccccc2C(C)(C)c2ccccc21
Mol. weight [g/mol]:	294.43
CAS:	4757-55-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	4.416		Crippen Method
mcpvol	254.240	ml/mol	McGowan Method
rinpol	2343.00		NIST Webbook
rinpol	2313.00		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=C4757555&Units=SI

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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