

Mequitazine

Other names:

10H-Phenothiazine, 10-(1-azabicyclo[2.2.2]oct-3-ylmethyl)-
LM 209
Phenothiazine, 10-(3-quinuclidinylmethyl)-
Virginan
10-(3-Quinuclidinylmethyl)phenothiazine
Instotal
Mequitazina
Metaplexan
Mircol
Primalan
Vigigan
Butix
Zesulan
10-(1-Azabicyclo[2.2.2]oct-3-ylmethyl)-10H-phenothiazine
NSC 303612

Inchi:

InChI=1S/C20H22N2S/c1-3-7-19-17(5-1)22(18-6-2-4-8-20(18)23-19)14-16-13-21-11-9-15

InchiKey:

HOKDBMAJZXIPGC-UHFFFAOYSA-N

Formula:

C20H22N2S

SMILES:

c1ccc2c(c1)Sc1cccc1N2CC1CN2CCC1CC2

Mol. weight [g/mol]:

322.47

CAS:

29216-28-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.631		Crippen Method
mcvol	248.870	ml/mol	McGowan Method
rinpol	2804.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2804.00		NIST Webbook
rinpol	2765.00		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=C29216282&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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<https://www.chemeo.com/cid/87-441-6/Mequitazine.pdf>

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