

Propionylpromazone

Other names:	1-Propanone, 1-[10-[3-(dimethylamino)propyl]-10H-phenothiazin-2-yl]- 1-Propanone, 1-[10-[3-(dimethylamino)propyl]phenothiazin-2-yl]- Bayer 188 Combelen Combilen Propionpromazine Propionylpromazine Propiopromazine 10-(3-Dimethylaminopropyl)-2-propionylphenothiazine 1497CB 2-Propionyl-10-(3-Dimethylaminopropyl)phenothiazine 2-Propionylpromazine BAY 188 1-(10-(3-(Dimethylamino)propyl)phenothiazin-2-yl)-1-propanone 1-[10-[3-(dimethylamino)propyl]-10H-phenothiazin-2-yl]propan-1-one
Inchi:	InChI=1S/C20H24N2OS/c1-4-18(23)15-10-11-20-17(14-15)22(13-7-12-21(2)3)16-8-5-6-9
InchiKey:	ZQTVCQIJTREKSP-UHFFFAOYSA-N
Formula:	C20H24N2OS
SMILES:	CCC(=O)c1ccc2c(c1)N(CCCN(C)C)c1cccc1S2
Mol. weight [g/mol]:	340.48
CAS:	3568-24-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.834		Crippen Method
mcvol	272.160	ml/mol	McGowan Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
rinpol	2804.00		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=C3568249&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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