

Propiomazine

Other names:

1-Propanone, 1-[10-[2-(dimethylamino)propyl]-10H-phenothiazin-2-yl]-
1-Propanone, 1-[10-[2-(dimethylamino)propyl]phenothiazin-2-yl]-
Propionylpromethazine
2-Propionyl-10-[2-(dimethylamino)propyl]phenothiazine
1-[10-[2-(Dimethylamino)propyl]phenothiazin-2-yl]-1-propanone
1-[10-[2-(Dimethylamino)propyl]-10H-phenothiazin-2-yl]-1-propanone
Wy-1359

Inchi: InChI=1S/C20H24N2OS/c1-5-18(23)15-10-11-20-17(12-15)22(13-14(2)21(3)4)16-8-6-7-9**InchiKey:** UVOIBTBFPOZKGP-UHFFFAOYSA-N**Formula:** C20H24N2OS**SMILES:** CCC(=O)c1ccc2c(c1)N(CC(C)N(C)C)c1ccccc1S2**Mol. weight [g/mol]:** 340.48**CAS:** 362-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	4.832		Crippen Method
mcvol	272.160	ml/mol	McGowan Method
rinpol	2738.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2736.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2736.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C362298&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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