

Acetophenazine

Other names:	Ethanone, 1-[10-[3-[4-(2-hydroxyethyl)-1-piperazinyl]propyl]-10H-phenothiazin-2-yl]- Ketone, 10-[3-[4-(2-hydroxyethyl)-1-piperazinyl]propyl]phenothiazin-2-yl methyl Acetophenazinum
Inchi:	InChI=1S/C23H29N3O2S/c1-18(28)19-7-8-23-21(17-19)26(20-5-2-3-6-22(20)29-23)10-4
InchiKey:	WNTYBHLDCCKXEOT-UHFFFAOYSA-N
Formula:	C23H29N3O2S
SMILES:	<chem>CC(=O)c1ccc2c(c1)N(CCCN1CCN(CCO)CC1)c1cccc1S2</chem>
Mol. weight [g/mol]:	411.56
CAS:	2751-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	3.492		Crippen Method
mcvol	319.420	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2751680&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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