

Butaperazine M (nor-), monoacetylated

Inchi:	InChI=1S/C25H31N3O2S/c1-3-7-23(30)20-10-11-25-22(18-20)28(21-8-4-5-9-24(21)31-2
InchiKey:	DGHSJBVTKGCPQK-UHFFFAOYSA-N
Formula:	C25H31N3O2S
SMILES:	CCCC(=O)c1ccc2c(c1)N(CCCN1CCN(C(C)=O)CC1)c1cccc1S2
Mol. weight [g/mol]:	437.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	4.826		Crippen Method
mcvol	343.300	ml/mol	McGowan Method
rinpol	3800.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R310160&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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<https://www.chemeo.com/cid/23-039-3/Butaperazine-M-nor-monoacetylated.pdf>

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