

Ketotifen M (nor), acetylated

Inchi:	InChI=1S/C20H19NO2S/c1-13(22)21-9-6-14(7-10-21)19-16-5-3-2-4-15(16)12-18(23)20-1
InchiKey:	DZZDDFWCAOAASM-UHFFFAOYSA-N
Formula:	C20H19NO2S
SMILES:	CC(=O)N1CCC(=C2c3ccccc3CC(=O)c3sc32)CC1
Mol. weight [g/mol]:	337.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	3.931		Crippen Method
mcvol	252.890	ml/mol	McGowan Method
rinsol	3180.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/16-869-0/Ketotifen-M-nor-acetylated.pdf>

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