

# Tritiozine

**Other names:**

Morpholine, 4-[thioxo(3,4,5-trimethoxyphenyl)methyl]-  
Morpholine, 4-(3,4,5-trimethoxythiobenzoyl)-  
ISF 2001  
Morpholine, 4-(thioxo(3,4,5-trimethoxyphenyl)methyl)-  
4-(Thioxo(3,4,5-trimethoxyphenyl)methyl)morpholine  
Tresanil  
Trithiozine  
4-(3,4,5-Trimethoxythiobenzoyl)morpholine  
4-(3,4,5-Trimethoxythiobenzoyl)tetrahydro-1,4-oxazine  
Tritiozina  
Sulmetozine

**Inchi:**

InChI=1S/C14H19NO4S/c1-16-11-8-10(9-12(17-2)13(11)18-3)14(20)15-4-6-19-7-5-15/h8

**InchiKey:**

MVOUIYUWRXPNKD-UHFFFAOYSA-N

**Formula:**

C14H19NO4S

**SMILES:**

COc1cc(C(=S)N2CCOCC2)cc(OC)c1OC

**Mol. weight [g/mol]:**

297.37

**CAS:**

35619-65-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.720		Crippen Method
mcvol	219.010	ml/mol	McGowan Method
rmpol	2396.00		NIST Webbook

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C35619659&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

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