

# 3-(3-Nitroanilinomethyl)-2-benzothiazolinethione

<b>Other names:</b>	2-Benzothiazolinethione, 3-[(m-nitroanilino)methyl]-
<b>Inchi:</b>	InChI=1S/C14H11N3O2S2/c18-17(19)11-5-3-4-10(8-11)15-9-16-12-6-1-2-7-13(12)21-14
<b>InchiKey:</b>	QXJUHNJHOMXNDT-UHFFFAOYSA-N
<b>Formula:</b>	C14H11N3O2S2
<b>SMILES:</b>	O=[N+](O-)c1cccc(NCn2c(=S)sc3ccccc32)c1
<b>Mol. weight [g/mol]:</b>	317.39
<b>CAS:</b>	65537-00-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	4.410		Crippen Method
mcvol	215.520	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C65537000&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C65537000&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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

Latest version available from:

<https://www.chemeo.com/cid/49-181-7/3-3-Nitroanilinomethyl-2-benzothiazolinethione.pdf>

Generated by Cheméo on 2024-04-19 02:08:26.71900822 +0000 UTC m=+15781755.639585537.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.