

# 2-Benzothiazolinethione, 3-(4-nitrophenylaminomethyl)-

Inchi:	InChI=1S/C14H11N3O2S2/c18-17(19)11-7-5-10(6-8-11)15-9-16-12-3-1-2-4-13(12)21-14
InchiKey:	UTKZLNADJQUIFU-UHFFFAOYSA-N
Formula:	C14H11N3O2S2
SMILES:	O=[N+]([O-])c1ccc(NCn2c(=S)sc3ccccc32)cc1
Mol. weight [g/mol]:	317.39
CAS:	60431-65-4

## 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

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C60431654&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60431654&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/119-871-3/2-Benzothiazolinethione-3-4-nitrophenylaminomethyl.pdf>

Generated by Cheméo on 2024-04-29 09:17:20.873322037 +0000 UTC m=+16671489.793899349.

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