

# 2-Mercapto-4-phenylthiazole

<b>Other names:</b>	2(3H)-Thiazolethione, 4-phenyl- 4-Phenyl-2-mercaptothiazole 4-Phenylthiazole-2-thiol 4-Thiazoline-2-thione, 4-phenyl- 4-phenylthiazole-2(3H)-thione
<b>Inchi:</b>	InChI=1S/C9H7NS2/c11-9-10-8(6-12-9)7-4-2-1-3-5-7/h1-6H,(H,10,11)
<b>InchiKey:</b>	CYCKHTAVNBPQDB-UHFFFAOYSA-N
<b>Formula:</b>	C9H7NS2
<b>SMILES:</b>	Sc1nc(-c2ccccc2)cs1
<b>Mol. weight [g/mol]:</b>	193.29
<b>CAS:</b>	2103-88-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.099		Crippen Method
mcvol	137.130	ml/mol	McGowan Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2103880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2103880&amp;Units=SI</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.cheméo.com/cid/57-163-8/2-Mercapto-4-phenylthiazole.pdf>

Generated by Cheméo on 2024-04-26 03:23:25.221683559 +0000 UTC m=+16391054.142260882.

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