

# Naphtho[1,2-d]thiazole, 2-methyl-

<b>Other names:</b>	2-Methyl-«beta»-naphthothiazole 2-methyl-.beta.-naphthothiazole 2-methylnaphtho[1,2-d]thiazole Naphth[1,2-d]thiazole, 2-methyl-
<b>Inchi:</b>	InChI=1S/C12H9NS/c1-8-13-12-10-5-3-2-4-9(10)6-7-11(12)14-8/h2-7H,1H3
<b>InchiKey:</b>	OUXMJRMYZCEVKO-UHFFFAOYSA-N
<b>Formula:</b>	C12H9NS
<b>SMILES:</b>	Cc1nc2c(ccc3ccccc32)s1
<b>Mol. weight [g/mol]:</b>	199.27
<b>CAS:</b>	2682-45-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	3.758		Crippen Method
mcvol	147.890	ml/mol	McGowan Method
tf	368.01	K	Thermodynamic properties of naphthoxazole and naphthothiazole derivatives: Experimental and computational studies

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Thermodynamic properties of naphthoxazole and naphthothiazole derivatives: Experimental and computational studies:</b>	<a href="https://www.doi.org/10.1016/j.jct.2018.07.008">https://www.doi.org/10.1016/j.jct.2018.07.008</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=C2682453&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2682453&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tf:** Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/60-547-8/Naphtho-1-2-d-thiazole-2-methyl.pdf>

Generated by Cheméo on 2024-04-20 01:56:08.564979928 +0000 UTC m=+15867417.485557241.

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