

# 11-Methylbenzo[b]naphtho[1,2-d]thiophene

<b>Other names:</b>	Benzo[b]naphtho[1,2-d]thiophene, 11-methyl Benzo[b]naphtho[1,2]thiophene, 11-methyl
<b>Inchi:</b>	InChI=1S/C17H12S/c1-11-5-4-8-14-16(11)17-13-7-3-2-6-12(13)9-10-15(17)18-14/h2-10H
<b>InchiKey:</b>	ZDMWKUISVKVZNB-UHFFFAOYSA-N
<b>Formula:</b>	C17H12S
<b>SMILES:</b>	Cc1cccc2sc3ccc4ccccc4c3c12
<b>Mol. weight [g/mol]:</b>	248.34
<b>CAS:</b>	84258-84-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	403.10		NIST Webbook
rinpol	404.15		NIST Webbook
rinpol	402.67		NIST Webbook

## Sources

<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=C84258844&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C84258844&amp;Units=SI</a>
<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>

## 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

Latest version available from:

<https://www.cheméo.com/cid/54-390-9/11-Methylbenzo-b-naphtho-1-2-d-thiophene.pdf>

Generated by Cheméo on 2024-04-17 14:38:40.270348881 +0000 UTC m=+15653969.190926196.

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