

# Naphtho[2,1-b]thiophene, 7-methyl

<b>Other names:</b>	7-Methylnaphtho[2,1-b]thiophene Naphtho[2.1-b]thiophene, 7-methyl
<b>Inchi:</b>	InChI=1S/C13H10S/c1-9-2-4-11-10(8-9)3-5-13-12(11)6-7-14-13/h2-8H,1H3
<b>InchiKey:</b>	SKDBEKIAJLSGPS-UHFFFAOYSA-N
<b>Formula:</b>	C13H10S
<b>SMILES:</b>	<chem>Cc1ccc2c(ccc3sccc32)c1</chem>
<b>Mol. weight [g/mol]:</b>	198.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	4.363		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
rinpol	320.50		NIST Webbook
rinpol	320.26		NIST Webbook
rinpol	317.67		NIST Webbook
rinpol	317.67		NIST Webbook

## 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=R21621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R21621&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
<b>rinpol:</b>	Non-polar retention indices

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