

# Benzo[2,3]phenanthro[4,5]thiophene, 9-methyl

<b>Inchi:</b>	InChI=1S/C19H12S/c1-11-5-6-13-10-14-8-7-12-3-2-4-16-17(12)18(14)19(20-16)15(13)9-
<b>InchiKey:</b>	XURXPZTUILTPNB-UHFFFAOYSA-N
<b>Formula:</b>	C19H12S
<b>SMILES:</b>	<chem>Cc1ccc2cc3ccc4cccc5sc(c2c1)c3c45</chem>
<b>Mol. weight [g/mol]:</b>	272.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	6.107		Crippen Method
mcvol	201.920	ml/mol	McGowan Method
rinpol	456.63		NIST Webbook
rinpol	456.63		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=R642536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R642536&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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

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