

# Triphenyleno-di[1,12-bcd:8,9-bcd]thiophene

<b>Inchi:</b>	InChI=1S/C18H8S2/c1-3-9-10-4-2-6-12-16(10)18-14(20-12)8-7-13-17(18)15(9)11(5-1)19
<b>InchiKey:</b>	FRRKTHIVLIBONP-UHFFFAOYSA-N
<b>Formula:</b>	C18H8S2
<b>SMILES:</b>	c1cc2sc3ccc4sc5cccc6c(c1)c2c3c4c56
<b>Mol. weight [g/mol]:</b>	288.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.84		Crippen Method
logp	6.451		Crippen Method
mcvol	193.320	ml/mol	McGowan Method
rinpol	497.90		NIST Webbook
rinpol	497.10		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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R186497&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R186497&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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