

# Pyreno[1,2]thiophene

<b>Inchi:</b>	InChI=1S/C18H10S/c1-2-11-4-5-13-10-14-8-9-19-18(14)15-7-6-12(3-1)16(11)17(13)15/h
<b>InchiKey:</b>	KCKFFTQULGAQPQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H10S
<b>SMILES:</b>	c1cc2ccc3cc4ccsc4c4ccc(c1)c2c34
<b>Mol. weight [g/mol]:</b>	258.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	5.799		Crippen Method
mcvol	187.830	ml/mol	McGowan Method
rinpol	446.18		NIST Webbook
rinpol	446.18		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=R643133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R643133&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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