

# Anthra[2,1-b]thiophene, 1-methyl

**Inchi:** InChI=1S/C20H12S/c1-2-6-14-12-18-15(11-13(14)5-1)9-10-17-16-7-3-4-8-19(16)21-20(1)  
**InchiKey:** PNOLZEWNRDUVGV-UHFFFAOYSA-N  
**Formula:** C20H12S  
**SMILES:** c1ccc2cc3c(ccc4c5ccccc5sc34)cc2c1  
**Mol. weight [g/mol]:** 284.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
rinpol	418.22		NIST Webbook
rinpol	418.22		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21087&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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