

# Anthra(2,1-b)thiophene

**Inchi:** InChI=1S/C16H10S/c1-2-4-12-10-15-13(9-11(12)3-1)5-6-16-14(15)7-8-17-16/h1-10H  
**InchiKey:** PAYSBLPSJQBEJR-UHFFFAOYSA-N  
**Formula:** C16H10S  
**SMILES:** c1ccc2cc3c(ccc4sccc43)cc2c1  
**Mol. weight [g/mol]:** 234.32  
**CAS:** 227-56-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	5.208		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
rinpol	399.06		NIST Webbook
rinpol	399.26		NIST Webbook
rinpol	399.31		NIST Webbook
rinpol	399.06		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=C227565&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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