

# Benzo[b]phenanthro[2,1-d]thiophene

**Inchi:** InChI=1S/C20H12S/c1-2-6-14-13(5-1)9-10-16-15(14)11-12-19-20(16)17-7-3-4-8-18(17)2  
**InchiKey:** XFWOYFBQPOFPRC-UHFFFAOYSA-N  
**Formula:** C20H12S  
**SMILES:** c1ccc2c(c1)ccc1c2ccc2sc3ccccc3c21  
**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	487.60		NIST Webbook
rinpol	482.50		NIST Webbook
rinpol	482.20		NIST Webbook
rinpol	482.30		NIST Webbook
rinpol	487.60		NIST Webbook
rinpol	488.89		NIST Webbook
rinpol	482.30		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=R21322&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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