

# Benzo[2,3]phenanthro[4,5-bcd]thiophene

**Other names:** Benzo[b]phenanthro[4,5-bcd]thiophene  
**Inchi:** InChI=1S/C18H10S/c1-2-6-14-12(4-1)10-13-9-8-11-5-3-7-15-16(11)17(13)18(14)19-15/h  
**InchiKey:** SVXCMFMVRIKHHD-UHFFFAOYSA-N  
**Formula:** C18H10S  
**SMILES:** c1ccc2c(c1)cc1ccc3cccc4sc2c1c34  
**Mol. weight [g/mol]:** 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	443.30		NIST Webbook
rinpol	443.74		NIST Webbook
rinpol	443.29		NIST Webbook
rinpol	436.00		NIST Webbook
rinpol	443.30		NIST Webbook
rinpol	436.00		NIST Webbook
rinpol	436.00		NIST Webbook
rinpol	434.70		NIST Webbook
rinpol	435.60		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=R21126&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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