

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

**Inchi:** InChI=1S/C20H12S/c1-2-6-14-13(5-1)9-10-17-15(14)11-12-18-16-7-3-4-8-19(16)21-20(1)  
**InchiKey:** SLVCPGQXYUUYDH-UHFFFAOYSA-N  
**Formula:** C20H12S  
**SMILES:** c1ccc2c(c1)ccc1c2ccc2c3ccccc3sc21  
**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	488.30		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	491.45		NIST Webbook
rinpol	491.20		NIST Webbook
rinpol	492.31		NIST Webbook
rinpol	491.45		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=R21318&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

Latest version available from:

<https://www.cheméo.com/cid/10-521-1/Benzo-b-phenanthro-1-2-d-thiophene.pdf>

Generated by Cheméo on 2024-04-25 19:48:50.080323504 +0000 UTC m=+16363779.000900826.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.