

# Benzo[4,5]phenaleno[9,1-bc]thiophene

**Inchi:** InChI=1S/C18H10S/c1-2-4-14-11(3-1)9-12-5-6-13-10-19-16-8-7-15(14)17(12)18(13)16/h  
**InchiKey:** QWQMZHGXBGJJBB-UHFFFAOYSA-N  
**Formula:** C18H10S  
**SMILES:** c1ccc2c(c1)cc1ccc3csc4ccc2c1c34  
**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	458.00		NIST Webbook
rinpol	457.30		NIST Webbook
rinpol	458.00		NIST Webbook

## Sources

**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=R21144&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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