# Benzo[b]naphtho[1,2-d]thiophene, 1-methyl

**Other names:** Benzo[b]naphtho[1,2]thiophene, 1-methyl
**Inchi:** InChI=1S/C17H12S/c1-11-5-4-6-12-9-10-15-17(16(11)12)13-7-2-3-8-14(13)18-15/h2-10H
**InchiKey:** WAKYXINVOCPQFY-UHFFFAOYSA-N
**Formula:** C17H12S
**SMILES:** Cc1cccc2ccc3sc4ccccc4c3c12
**Mol. weight [g/mol]:** 248.34
**CAS:** 84258-62-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.12 | | Crippen Method |
| logp | 5.516 | | Crippen Method |
| mcvol | 188.900 | ml/mol | McGowan Method |
| rinpol | 400.83 | | NIST Webbook |
| rinpol | 400.83 | | NIST Webbook |
| rinpol | 402.59 | | NIST Webbook |
| rinpol | 402.59 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C84258628&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices