

Benzo[b]naphtho[2,3]thiophene, 4-methyl

| | |
|-----------------------------|---|
| Other names: | Benzo[b]naphtho[2,3-d]thiophene, 4-methyl |
| Inchi: | InChI=1S/C17H12S/c1-11-5-4-8-14-15-9-12-6-2-3-7-13(12)10-16(15)18-17(11)14/h2-10H |
| InchiKey: | YTNVYFJVEVMZDG-UHFFFAOYSA-N |
| Formula: | C17H12S |
| SMILES: | <chem>Cc1cccc2c1sc1cc3ccccc3cc12</chem> |
| Mol. weight [g/mol]: | 248.34 |
| CAS: | 36821-08-6 |

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 | 411.60 | | NIST Webbook |
| rinpol | 410.66 | | NIST Webbook |
| rinpol | 411.60 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C36821086&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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/35-234-3/Benzo-b-naphtho-2-3-thiophene-4-methyl.pdf>

Generated by Cheméo on 2024-04-19 17:21:10.306407202 +0000 UTC m=+15836519.226984514.

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