

Pyreno[2,1]thiophene

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|-----------------------------|---|
| Inchi: | InChI=1S/C18H10S/c1-2-11-4-5-13-10-16-14(8-9-19-16)15-7-6-12(3-1)17(11)18(13)15/h |
| InchiKey: | KBGGQFXUYZPGSX-UHFFFAOYSA-N |
| Formula: | C18H10S |
| SMILES: | c1cc2ccc3cc4sccc4c4ccc(c1)c2c34 |
| 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 | 451.56 | | NIST Webbook |
| rinpol | 451.56 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R643148&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.chemeo.com/cid/78-244-5/Pyreno-2-1-thiophene.pdf>

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