

Naphtho[1,2-b]thiophene, 2-methyl

Inchi: InChI=1S/C13H10S/c1-9-8-11-7-6-10-4-2-3-5-12(10)13(11)14-9/h2-8H,1H3
InchiKey: RJAPHDMCOJKTEQ-UHFFFAOYSA-N
Formula: C13H10S
SMILES: Cc1cc2ccc3ccccc3c2s1
Mol. weight [g/mol]: 198.28

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.31 | | Crippen Method |
| logp | 4.363 | | Crippen Method |
| mcvol | 152.000 | ml/mol | McGowan Method |
| rinpol | 312.11 | | NIST Webbook |
| rinpol | 312.11 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R193029&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

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<https://www.chemeo.com/cid/24-304-7/Naphtho-1-2-b-thiophene-2-methyl.pdf>

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