

Thiophene, 3-ethyl-2-methyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C7H10S/c1-3-7-4-5-8-6(7)2/h4-5H,3H2,1-2H3 |
| InchiKey: | RBRAJDCWXUJHIY-UHFFFAOYSA-N |
| Formula: | C7H10S |
| SMILES: | CCc1ccsc1C |
| Mol. weight [g/mol]: | 126.22 |
| CAS: | 53119-51-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.51 | | Crippen Method |
| logp | 2.619 | | Crippen Method |
| mcvol | 106.380 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=C53119510&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

Latest version available from:

<https://www.chemeo.com/cid/73-113-5/Thiophene-3-ethyl-2-methyl.pdf>

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