

3-Thiophenemethanol

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|-----------------------------|--|
| Other names: | Thiophene-3-methanol 3-Thienylmethanol |
| Inchi: | InChI=1S/C5H6OS/c6-3-5-1-2-7-4-5/h1-2,4,6H,3H2 |
| InchiKey: | BOWIFWCBNWWZOG-UHFFFAOYSA-N |
| Formula: | C5H6OS |
| SMILES: | OCc1ccsc1 |
| Mol. weight [g/mol]: | 114.17 |
| CAS: | 71637-34-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.37 | | Crippen Method |
| logp | 1.240 | | Crippen Method |
| mcvol | 84.070 | ml/mol | McGowan Method |
| rinpol | 1052.00 | | NIST Webbook |
| rinpol | 1052.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C71637348&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.chemeo.com/cid/41-793-6/3-Thiophenemethanol.pdf>

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