

3-Thenyl bromide

| | |
|-----------------------------|---|
| Other names: | 3-(bromomethyl)thiophene |
| Inchi: | InChI=1S/C5H5BrS/c6-3-5-1-2-7-4-5/h1-2,4H,3H2 |
| InchiKey: | KBWHYRUAHXHHFO-UHFFFAOYSA-N |
| Formula: | C5H5BrS |
| SMILES: | BrCc1ccsc1 |
| Mol. weight [g/mol]: | 177.06 |
| CAS: | 34846-44-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -2.54 | | Crippen Method |
| logp | 2.643 | | Crippen Method |
| mcvol | 95.700 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C34846441&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

Latest version available from:

<https://www.chemeo.com/cid/80-840-0/3-Thenyl-bromide.pdf>

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