

2-Thiopheneethanol

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|-----------------------------|---|
| Other names: | 2-(2-Thienyl)ethanol 2-(2-Hydroxyethyl)thiophene Thiophene-2-ethanol Thiopheneethanol Ethanol, 2-(2-thienyl)- thiophen-2-ethanol |
| Inchi: | InChI=1S/C6H8OS/c7-4-3-6-2-1-5-8-6/h1-2,5,7H,3-4H2 |
| InchiKey: | VMJOFTHFJMLIKL-UHFFFAOYSA-N |
| Formula: | C6H8OS |
| SMILES: | OCCc1cccs1 |
| Mol. weight [g/mol]: | 128.19 |
| CAS: | 5402-55-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -1.30 | | Crippen Method |
| logp | 1.283 | | Crippen Method |
| mcvol | 98.160 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 381.70 | K | 1.70 | 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=C5402551&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tbrp: | Boiling point at reduced pressure |

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