

Thiophene, 2-(phenylmethyl)-

| | |
|-----------------------------|---|
| Other names: | Thiophene, 2-benzyl- 2-Benzylthiophene |
| Inchi: | InChI=1S/C11H10S/c1-2-5-10(6-3-1)9-11-7-4-8-12-11/h1-8H,9H2 |
| InchiKey: | VPGIYLLXBOUILV-UHFFFAOYSA-N |
| Formula: | C11H10S |
| SMILES: | <chem>c1ccc(Cc2cccs2)cc1</chem> |
| Mol. weight [g/mol]: | 174.26 |
| CAS: | 13132-15-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.33 | | Crippen Method |
| logp | 3.339 | | Crippen Method |
| mcvol | 138.980 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 348.00 | K | 0.02 | NIST Webbook |

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=C13132155&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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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