

2-Acetyl-5-methylthiophene

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|-----------------------------|---|
| Other names: | Methyl 5-methyl-2-thienyl ketone Ethanone, 1-(5-methyl-2-thienyl)- Ketone, methyl 5-methyl-2-thienyl 2-Methyl-5-acetylthiophene 1-(5-Methyl-2-thienyl)ethanone 5-Methyl-2-acetylthiophene Thiophene, 2-acetyl-5-methyl 1-(5-methyl-2-thienyl)ethan-1-one |
| Inchi: | InChI=1S/C7H8OS/c1-5-3-4-7(9-5)6(2)8/h3-4H,1-2H3 |
| InchiKey: | YOSDTJYMDAEEAZ-UHFFFAOYSA-N |
| Formula: | C7H8OS |
| SMILES: | CC(=O)c1ccc(C)s1 |
| Mol. weight [g/mol]: | 140.20 |
| CAS: | 13679-74-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|--------|----------------|
| hvap | 62.00 ± 2.60 | kJ/mol | NIST Webbook |
| log10ws | -2.36 | | Crippen Method |
| logp | 2.259 | | Crippen Method |
| mcvol | 107.950 | ml/mol | McGowan Method |
| rinpol | 1185.00 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1157.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| rinpol | 1123.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1197.00 | | NIST Webbook |
| rinpol | 1185.00 | | NIST Webbook |
| rinpol | 1170.00 | | NIST Webbook |
| rinpol | 1174.00 | | NIST Webbook |
| ripol | 1914.00 | | NIST Webbook |
| ripol | 1874.00 | | NIST Webbook |
| ripol | 1914.00 | | NIST Webbook |
| ripol | 1836.00 | | NIST Webbook |
| tb | 505.50 ± 0.50 | K | NIST Webbook |
| tb | 505.70 | K | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 372.20 | K | 1.00 | NIST Webbook |
| tbrp | 372.00 ± 1.00 | K | 1.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679748&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tf: | Normal melting (fusion) point |

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