# 2-ACETYL-5-CHLOROTHIOPHENE

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|---|---|
| **Other names:** | 5-Chloro-2-thienyl methyl ketone |
| | Ethanone, 1-(5-chloro-2-thienyl)- |
| | Ketone, 5-chloro-2-thienyl methyl |
| | BA 11044 |
| | 5-Chlor-2-acetyl thiophen |
| | 5-Chloro-2-acetyl thiophen |
| | 1-(5-Chloro-2-thienyl)ethanone |
| | 2-Chloro-5-acetylthiophene |
| | 5-Chloro-2-acetylthiophene |
| | NSC 43020 |
| | 1-(5-chloro-2-thienyl)ethan-1-one |
| **Inchi:** | InChI=1S/C6H5ClOS/c1-4(8)5-2-3-6(7)9-5/h2-3H,1H3 |
| **InchiKey:** | HTZGPEHWQCRXGZ-UHFFFAOYSA-N |
| **Formula:** | C6H5ClOS |
| **SMILES:** | CC(=O)c1ccc(Cl)s1 |
| **Mol. weight [g/mol]:** | 160.63 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hvap | 61.57 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.16 | eV | Cheméo Relay (1.0) |
| logp | 2.604 | | Crippen Method |
| mcvol | 106.100 | ml/mol | McGowan Method |
| tb | 494.16 | K | Cheméo Relay (1.0) |
| tf | 347.01 | K | Cheméo Relay (1.0) |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 390.70 | K | 2.30 | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6310094&Units=SI |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

# Legend

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|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tf:** | Normal melting (fusion) point |