

# 4-Hydroxy-5-methyl-3(2H)thiophenone

**Inchi:** InChI=1S/C6H8OS/c1-4-5(2)8-3-6(4)7/h3H2,1-2H3  
**InchiKey:** FVRWQHLYVNTARH-UHFFFAOYSA-N  
**Formula:** C6H8OS  
**SMILES:** CC1=C(C)C(=O)CS1  
**Mol. weight [g/mol]:** 128.19

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -28.13  | kJ/mol  | Joback Method  |
| hf            | -143.95 | kJ/mol  | Joback Method  |
| hfus          | 7.77    | kJ/mol  | Joback Method  |
| hvap          | 41.19   | kJ/mol  | Joback Method  |
| log10ws       | -1.74   |         | Crippen Method |
| logp          | 1.596   |         | Crippen Method |
| mcvol         | 98.160  | ml/mol  | McGowan Method |
| pc            | 4183.90 | kPa     | Joback Method  |
| rinpol        | 879.00  |         | NIST Webbook   |
| rinpol        | 879.00  |         | NIST Webbook   |
| tb            | 481.40  | K       | Joback Method  |
| tc            | 720.36  | K       | Joback Method  |
| tf            | 349.99  | K       | Joback Method  |
| vc            | 0.352   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 191.02 | J/mol×K | 481.40          | Joback Method |
| cpg           | 201.89 | J/mol×K | 521.23          | Joback Method |
| cpg           | 212.30 | J/mol×K | 561.05          | Joback Method |
| cpg           | 222.23 | J/mol×K | 600.88          | Joback Method |
| cpg           | 231.67 | J/mol×K | 640.71          | Joback Method |
| cpg           | 240.62 | J/mol×K | 680.54          | Joback Method |
| cpg           | 249.07 | J/mol×K | 720.36          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R618305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R618305&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvac:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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