# 4-(METHYLTHIO)ACETOPHENONE

**Other names:** 4-(Methylthio)acetophenone
4-CH3S-C6H4-COCH3
1-[4-(methylthio)phenyl]ethan-1-one
**Inchi:** InChI=1S/C9H10OS/c1-7(10)8-3-5-9(11-2)6-4-8/h3-6H,1-2H3
**InchiKey:** JECUZQLBQKNEMW-UHFFFAOYSA-N
**Formula:** C9H10OS
**SMILES:** CSc1ccc(C(C)=O)cc1
**Mol. weight [g/mol]:** 166.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4299 | | Cheméo Relay (1.0) |
| affp | 888.20 | kJ/mol | NIST Webbook |
| basg | 856.30 | kJ/mol | NIST Webbook |
| gf | 31.88 | kJ/mol | Joback Method |
| hf | -100.99 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 18.45 | kJ/mol | Joback Method |
| hvap | 76.99 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.53 | eV | Cheméo Relay (1.0) |
| log10ws | -2.78 | | Cheméo Relay (1.0) |
| logp | 2.611 | | Crippen Method |
| mcvol | 131.830 | ml/mol | McGowan Method |
| pc | 3517.91 | kPa | Joback Method |
| tb | 552.93 | K | Cheméo Relay (1.0) |
| tc | 751.22 | K | Cheméo Relay (1.0) |
| tf | 329.81 | K | Cheméo Relay (1.0) |
| vc | 0.465 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 280.71 | J/mol×K | 559.63 | Joback Method |
| cpg | 293.43 | J/mol×K | 599.76 | Joback Method |
| cpg | 305.31 | J/mol×K | 639.90 | Joback Method |

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|---|---|---|---|---|
| cpg | 316.36 | J/mol×K | 680.03 | Joback Method |
| cpg | 326.60 | J/mol×K | 720.17 | Joback Method |
| cpg | 336.07 | J/mol×K | 760.30 | Joback Method |
| cpg | 344.78 | J/mol×K | 800.44 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1778092&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**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):**

# Legend

**af:** Acentric Factor
**affp:** Proton affinity
**basg:** Gas basicity
**cpg:** Ideal gas heat capacity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.