# 1-(Methylthio)-3-pentanone

**Other names:** 3-Pentanone, 1-(methylthio)-
1-(Methylthio)pentan-3-one
**Inchi:** InChI=1S/C6H12OS/c1-3-6(7)4-5-8-2/h3-5H2,1-2H3
**InchiKey:** LEZZIANNWFYCND-UHFFFAOYSA-N
**Formula:** C6H12OS
**SMILES:** CCC(=O)CCSC
**Mol. weight [g/mol]:** 132.22
**CAS:** 66735-69-1

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -96.16 | kJ/mol | Joback Method |
| hf | -237.88 | kJ/mol | Joback Method |
| hfus | 17.03 | kJ/mol | Joback Method |
| hvap | 42.51 | kJ/mol | Joback Method |
| log10ws | -1.50 | | Crippen Method |
| logp | 1.719 | | Crippen Method |
| mcvol | 113.320 | ml/mol | McGowan Method |
| pc | 3403.91 | kPa | Joback Method |
| rinpol | 1052.00 | | NIST Webbook |
| rinpol | 1045.00 | | NIST Webbook |
| rinpol | 1052.00 | | NIST Webbook |
| rinpol | 1045.00 | | NIST Webbook |
| rinpol | 1080.00 | | NIST Webbook |
| rinpol | 1080.00 | | NIST Webbook |
| ripol | 1570.00 | | NIST Webbook |
| ripol | 1593.00 | | NIST Webbook |
| ripol | 1588.00 | | NIST Webbook |
| ripol | 1588.00 | | NIST Webbook |
| ripol | 1593.00 | | NIST Webbook |
| tb | 459.33 | K | Joback Method |
| tc | 660.04 | K | Joback Method |
| tf | 241.71 | K | Joback Method |
| vc | 0.431 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 223.40 | J/mol×K | 459.33 | Joback Method |
| cpg | 234.25 | J/mol×K | 492.78 | Joback Method |
| cpg | 244.63 | J/mol×K | 526.23 | Joback Method |
| cpg | 254.54 | J/mol×K | 559.69 | Joback Method |
| cpg | 264.00 | J/mol×K | 593.14 | Joback Method |
| cpg | 273.01 | J/mol×K | 626.59 | Joback Method |
| cpg | 281.57 | J/mol×K | 660.04 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C66735691&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**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
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume