# Methyl 3-(methylthio)-(E)-2-propenoate

**Other names:** (E)-2-Propenoic acid, 3-methylthio-, methyl ester
Methyl 3-(methylthio)-2-propenoate, (E)
**Inchi:** InChI=1S/C5H8O2S/c1-7-5(6)3-4-8-2/h3-4H,1-2H3/b4-3+
**InchiKey:** KAFIOMPFBSDFPP-ONEGZZNKSA-N
**Formula:** C5H8O2S
**SMILES:** COC(=O)C=CSC
**Mol. weight [g/mol]:** 132.18
**CAS:** 15904-85-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -129.36 | kJ/mol | Joback Method |
| hf | -232.24 | kJ/mol | Joback Method |
| hfus | 15.82 | kJ/mol | Joback Method |
| hvap | 42.66 | kJ/mol | Joback Method |
| log10ws | -1.01 | | Crippen Method |
| logp | 1.036 | | Crippen Method |
| mcvol | 100.800 | ml/mol | McGowan Method |
| pc | 3990.60 | kPa | Joback Method |
| rinpol | 1062.00 | | NIST Webbook |
| ripol | 1663.00 | | NIST Webbook |
| ripol | 1675.00 | | NIST Webbook |
| tb | 463.03 | K | Joback Method |
| tc | 675.06 | K | Joback Method |
| tf | 247.59 | K | Joback Method |
| vc | 0.373 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 188.44 | J/mol×K | 463.03 | Joback Method |
| cpg | 197.25 | J/mol×K | 498.37 | Joback Method |
| cpg | 205.66 | J/mol×K | 533.71 | Joback Method |
| cpg | 213.69 | J/mol×K | 569.05 | Joback Method |

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|---|---|---|---|---|
| cpg | 221.33 | J/mol×K | 604.38 | Joback Method |
| cpg | 228.58 | J/mol×K | 639.72 | Joback Method |
| cpg | 235.46 | J/mol×K | 675.06 | 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=C15904855&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 |