# Thiirane, methyl-

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|---|---|
| **Other names:** | 1,2-Epithiopropane |
| | 2-Methylthiacyclopropane |
| | 2-Methylthiirane |
| | Methylthiirane |
| | NSC 36643 |
| | NSC 48100 |
| | Propane, 1,2-epithio- |
| | Propene sulfide |
| | Propylene episulfide |
| | Propylene sulfide |
| | Propylene sulphide |
| | Thiirane, 2-methyl- |
| **Inchi:** | InChI=1S/C3H6S/c1-3-2-4-3/h3H,2H2,1H3 |
| **InchiKey:** | MBNVSWHUJDDZRH-UHFFFAOYSA-N |
| **Formula:** | C3H6S |
| **SMILES:** | CC1CS1 |
| **Mol. weight [g/mol]:** | 74.14 |
| **CAS:** | 1072-43-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 833.30 | kJ/mol | NIST Webbook |
| basg | 801.50 | kJ/mol | NIST Webbook |
| chl | -2651.60 | kJ/mol | NIST Webbook |
| gf | 74.99 | kJ/mol | Joback Method |
| hf | 11.00 ± 1.00 | kJ/mol | NIST Webbook |
| hfus | 5.32 | kJ/mol | Joback Method |
| hvap | 28.00 | kJ/mol | Joback Method |
| ie | 8.60 ± 0.20 | eV | NIST Webbook |
| ie | 8.70 | eV | NIST Webbook |
| ie | 8.85 | eV | NIST Webbook |
| ie | 8.88 | eV | NIST Webbook |
| log10ws | -0.97 | | Crippen Method |
| logp | 1.122 | | Crippen Method |
| mcvol | 58.620 | ml/mol | McGowan Method |
| pc | 5235.81 | kPa | Joback Method |
| rinpol | 606.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 619.00 | | NIST Webbook |
| rinpol | 651.00 | | NIST Webbook |
| rinpol | 659.00 | | NIST Webbook |
| rinpol | 651.00 | | NIST Webbook |
| rinpol | 650.00 | | NIST Webbook |
| rinpol | 652.00 | | NIST Webbook |
| rinpol | 659.00 | | NIST Webbook |
| rinpol | 637.00 | | NIST Webbook |
| rinpol | 650.00 | | NIST Webbook |
| ripol | 924.00 | | NIST Webbook |
| ripol | 900.00 | | NIST Webbook |
| ripol | 915.00 | | NIST Webbook |
| ripol | 924.00 | | NIST Webbook |
| ripol | 875.00 | | NIST Webbook |
| tb | 345.70 | K | NIST Webbook |
| tc | 520.84 | K | Joback Method |
| tf | 224.96 | K | Joback Method |
| vc | 0.206 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 118.64 | J/mol×K | 487.80 | Joback Method |
| cpg | 83.33 | J/mol×K | 322.61 | Joback Method |
| cpg | 91.37 | J/mol×K | 355.65 | Joback Method |
| cpg | 98.89 | J/mol×K | 388.69 | Joback Method |
| cpg | 105.92 | J/mol×K | 421.72 | Joback Method |
| cpg | 112.50 | J/mol×K | 454.76 | Joback Method |
| cpg | 124.38 | J/mol×K | 520.84 | Joback Method |
| hvapt | 34.60 | kJ/mol | 347.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42819e+01 |
| Coeff. B | -2.87409e+03 |

| | |
|---|---|
| Coeff. C | -4.82860e+01 |
| Temperature range (K), min. | 253.66 |
| Temperature range (K), max. | 371.18 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072431&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor 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 |

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