# Methyl n-octyl sulfide

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|---|---|
| **Other names:** | 2-Thiadecane |
| | Octane, 1-(methylthio)- |
| | Octyl methyl sulfide |
| | methyl octyl sulphide |
| **Inchi:** | InChI=1S/C9H20S/c1-3-4-5-6-7-8-9-10-2/h3-9H2,1-2H3 |
| **InchiKey:** | AHCJTMBRROLNHV-UHFFFAOYSA-N |
| **Formula:** | C9H20S |
| **SMILES:** | CCCCCCCCSC |
| **Mol. weight [g/mol]:** | 160.32 |
| **CAS:** | 3698-95-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 58.02 | kJ/mol | Joback Method |
| hf | -187.22 | kJ/mol | Joback Method |
| hfus | 23.20 | kJ/mol | Joback Method |
| hvap | 42.45 | kJ/mol | Joback Method |
| log10ws | -3.47 | | Crippen Method |
| logp | 3.710 | | Crippen Method |
| mcvol | 154.020 | ml/mol | McGowan Method |
| pc | 2345.09 | kPa | Joback Method |
| rinpol | 1217.00 | | NIST Webbook |
| rinpol | 1217.00 | | NIST Webbook |
| ripol | 1426.30 | | NIST Webbook |
| ripol | 1431.70 | | NIST Webbook |
| ripol | 1453.00 | | NIST Webbook |
| tb | 474.10 | K | Joback Method |
| tc | 657.88 | K | Joback Method |
| tf | 225.59 | K | Joback Method |
| vc | 0.594 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 330.44 | J/mol×K | 474.10 | Joback Method |
| cpg | 345.32 | J/mol×K | 504.73 | Joback Method |
| cpg | 359.59 | J/mol×K | 535.36 | Joback Method |
| cpg | 373.27 | J/mol×K | 565.99 | Joback Method |
| cpg | 386.37 | J/mol×K | 596.62 | Joback Method |
| cpg | 398.90 | J/mol×K | 627.25 | Joback Method |
| cpg | 410.88 | J/mol×K | 657.88 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.71675e+01 |
| Coeff. B | -4.91594e+03 |
| Coeff. C | -7.76900e+01 |
| Temperature range (K), min. | 368.92 |
| Temperature range (K), max. | 492.33 |

# Sources

**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=C3698951&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

# 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

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|---|---|
| **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 |