# Hexane, 1-(methylthio)-

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|---|---|
| **Other names:** | 1-(Methylsulfanyl)hexane |
| | 1-(Methylthio)-hexane |
| | 2-Thiaoctane |
| | Hexyl methyl sulfide |
| | Sulfide, hexyl methyl |
| | n-Hexyl methyl sulfide |
| **Inchi:** | InChI=1S/C7H16S/c1-3-4-5-6-7-8-2/h3-7H2,1-2H3 |
| **InchiKey:** | LZRXQHHKXDXOIC-UHFFFAOYSA-N |
| **Formula:** | C7H16S |
| **SMILES:** | CCCCCCSC |
| **Mol. weight [g/mol]:** | 132.27 |
| **CAS:** | 20291-60-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 41.18 | kJ/mol | Joback Method |
| hf | -145.94 | kJ/mol | Joback Method |
| hfus | 18.02 | kJ/mol | Joback Method |
| hvap | 37.99 | kJ/mol | Joback Method |
| log10ws | -2.64 | | Crippen Method |
| logp | 2.930 | | Crippen Method |
| mcvol | 125.840 | ml/mol | McGowan Method |
| pc | 2850.52 | kPa | Joback Method |
| rinpol | 1004.00 | | NIST Webbook |
| rinpol | 1004.00 | | NIST Webbook |
| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1016.00 | | NIST Webbook |
| rinpol | 1004.00 | | NIST Webbook |
| ripol | 1251.00 | | NIST Webbook |
| ripol | 1232.10 | | NIST Webbook |
| ripol | 1232.10 | | NIST Webbook |
| ripol | 1227.00 | | NIST Webbook |
| tb | 428.34 | K | Joback Method |
| tc | 615.63 | K | Joback Method |
| tf | 206.35 ± 0.30 | K | NIST Webbook |
| vc | 0.481 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 245.59 | J/mol×K | 428.34 | Joback Method |
| cpg | 258.33 | J/mol×K | 459.56 | Joback Method |
| cpg | 270.58 | J/mol×K | 490.77 | Joback Method |
| cpg | 282.33 | J/mol×K | 521.99 | Joback Method |
| cpg | 293.61 | J/mol×K | 553.20 | Joback Method |
| cpg | 304.41 | J/mol×K | 584.42 | Joback Method |
| cpg | 314.75 | J/mol×K | 615.63 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.61352e+01 |
| Coeff. B | -4.19159e+03 |
| Coeff. C | -6.34510e+01 |
| Temperature range (K), min. | 327.94 |
| Temperature range (K), max. | 450.71 |

# 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=C20291605&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 |
| **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 |