# 1-Hexanethiol

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|---|---|
| **Other names:** | 1-Hexylthiol |
| | Hexan-1-thiol |
| | Hexanethiol |
| | Hexyl mercaptan |
| | N-HEXYL MERCAPTAN |
| | N-HEXYLTHIOL |
| | USAF EK-4628 |
| | hexane-1-thiol |
| | n-Hexanethiol |
| **Inchi:** | InChI=1S/C6H14S/c1-2-3-4-5-6-7/h7H,2-6H2,1H3 |
| **InchiKey:** | PMBXCGGQNSVESQ-UHFFFAOYSA-N |
| **Formula:** | C6H14S |
| **SMILES:** | CCCCCCS |
| **Mol. weight [g/mol]:** | 118.24 |
| **CAS:** | 111-31-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4788.50 ± 0.75 | kJ/mol | NIST Webbook |
| gf | 29.03 | kJ/mol | Joback Method |
| hf | -129.30 ± 0.96 | kJ/mol | NIST Webbook |
| hfl | -175.70 ± 0.92 | kJ/mol | NIST Webbook |
| hfus | 15.34 | kJ/mol | Joback Method |
| hvap | 44.80 ± 0.20 | kJ/mol | NIST Webbook |
| hvap | 46.40 | kJ/mol | NIST Webbook |
| log10ws | -2.41 | | Crippen Method |
| logp | 2.497 | | Crippen Method |
| mcvol | 111.750 | ml/mol | McGowan Method |
| pc | 3341.24 | kPa | Joback Method |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 927.30 | | NIST Webbook |
| rinpol | 912.50 | | NIST Webbook |
| rinpol | 920.90 | | NIST Webbook |
| rinpol | 920.40 | | NIST Webbook |
| rinpol | 922.00 | | NIST Webbook |
| rinpol | 925.00 | | NIST Webbook |
| rinpol | 918.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 930.00 | | NIST Webbook |
| rinpol | 929.00 | | NIST Webbook |
| rinpol | 917.00 | | NIST Webbook |
| rinpol | 904.00 | | NIST Webbook |
| rinpol | 918.00 | | NIST Webbook |
| rinpol | 904.00 | | NIST Webbook |
| rinpol | 930.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 927.00 | | NIST Webbook |
| rinpol | 912.00 | | NIST Webbook |
| rinpol | 916.00 | | NIST Webbook |
| rinpol | 903.00 | | NIST Webbook |
| rinpol | 901.00 | | NIST Webbook |
| rinpol | 908.00 | | NIST Webbook |
| rinpol | 909.00 | | NIST Webbook |
| rinpol | 909.00 | | NIST Webbook |
| rinpol | 910.00 | | NIST Webbook |
| rinpol | 920.00 | | NIST Webbook |
| rinpol | 916.40 | | NIST Webbook |
| ripol | 1145.00 | | NIST Webbook |
| ripol | 1145.00 | | NIST Webbook |
| ripol | 1153.20 | | NIST Webbook |
| ripol | 1153.20 | | NIST Webbook |
| ripol | 1165.00 | | NIST Webbook |
| ripol | 1140.00 | | NIST Webbook |
| ripol | 1165.00 | | NIST Webbook |
| ripol | 1148.00 | | NIST Webbook |
| sl | 343.21 | J/mol×K | NIST Webbook |
| tb | 420.00 ± 2.00 | K | NIST Webbook |
| tb | 422.85 | K | KDB |
| tb | 424.20 | K | NIST Webbook |
| tb | 425.75 ± 0.20 | K | NIST Webbook |
| tc | 588.15 | K | Joback Method |
| tf | 192.20 ± 0.30 | K | NIST Webbook |
| tf | 192.12 ± 0.30 | K | NIST Webbook |
| tf | 192.66 ± 0.02 | K | NIST Webbook |
| tt | 192.62 ± 0.02 | K | NIST Webbook |
| vc | 0.425 | m3/kmol | Joback Method |

# Temperature Dependent Properties

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

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|---|---|---|---|---|
| cpg | 204.81 | J/mol×K | 399.54 | Joback Method |
| cpg | 266.84 | J/mol×K | 588.15 | Joback Method |
| cpg | 257.60 | J/mol×K | 556.72 | Joback Method |
| cpg | 247.94 | J/mol×K | 525.28 | Joback Method |
| cpg | 237.85 | J/mol×K | 493.85 | Joback Method |
| cpg | 227.30 | J/mol×K | 462.41 | Joback Method |
| cpg | 216.29 | J/mol×K | 430.98 | Joback Method |
| cpl | 230.68 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 230.71 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 18.03 | kJ/mol | 192.60 | NIST Webbook |
| hfust | 18.03 | kJ/mol | 192.60 | NIST Webbook |
| hfust | 18.01 | kJ/mol | 192.62 | NIST Webbook |
| hvapt | 42.40 | kJ/mol | 410.00 | NIST Webbook |
| hvapt | 43.90 | kJ/mol | 387.00 | NIST Webbook |
| sfust | 93.51 | J/mol×K | 192.62 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55981e+01 |
| Coeff. B | -4.00405e+03 |
| Coeff. C | -5.95250e+01 |
| Temperature range (K), min. | 321.05 |
| Temperature range (K), max. | 448.77 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.11148e+01 |
| Coeff. B | -8.11731e+03 |
| Coeff. C | -9.63481e+00 |
| Coeff. D | 4.93320e-06 |
| Temperature range (K), min. | 192.62 |
| Temperature range (K), max. | 623.00 |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1834.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C111319&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1834 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |