# 2-Propanethiol

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|---|---|
| **Other names:** | 1-Methylethanethiol |
| | 2-MERCAPTOPROPANOL |
| | 2-Mercaptopropane |
| | 2-Propylmercaptan |
| | 2-Propylthiol |
| | ISO-PROPYL MERCAPTAN |
| | ISOPROPYLTHIOL |
| | Isopropanethiol |
| | Isopropyl mercaptan |
| | NSC 87537 |
| | Propanethiol-(2) |
| | iso-C3H7SH |
| | propane-2-thiol |
| **Inchi:** | InChI=1S/C3H8S/c1-3(2)4/h3-4H,1-2H3 |
| **InchiKey:** | KJRCEJOSASVSRA-UHFFFAOYSA-N |
| **Formula:** | C3H8S |
| **SMILES:** | CC(C)S |
| **Mol. weight [g/mol]:** | 76.16 |
| **CAS:** | 75-33-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 803.60 | kJ/mol | NIST Webbook |
| basg | 772.30 | kJ/mol | NIST Webbook |
| chl | -2819.30 ± 0.48 | kJ/mol | NIST Webbook |
| gf | 1.33 | kJ/mol | Joback Method |
| hf | -76.94 ± 0.63 | kJ/mol | NIST Webbook |
| hfl | -106.60 ± 0.63 | kJ/mol | NIST Webbook |
| hfus | 4.04 | kJ/mol | Joback Method |
| hvap | 30.10 | kJ/mol | NIST Webbook |
| hvap | 29.50 | kJ/mol | NIST Webbook |
| hvap | 29.70 | kJ/mol | NIST Webbook |
| hvap | 29.45 | kJ/mol | NIST Webbook |
| hvap | 29.63 | kJ/mol | NIST Webbook |
| ie | 9.15 | eV | NIST Webbook |
| ie | 9.15 | eV | NIST Webbook |
| ie | 9.14 | eV | NIST Webbook |

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|---|---|---|---|
| log10ws | -1.26 | | Crippen Method |
| logp | 1.325 | | Crippen Method |
| mcvol | 69.480 | ml/mol | McGowan Method |
| pc | 4862.97 | kPa | Joback Method |
| rinpol | 570.00 | | NIST Webbook |
| rinpol | 539.00 | | NIST Webbook |
| rinpol | 569.00 | | NIST Webbook |
| rinpol | 539.00 | | NIST Webbook |
| rinpol | 572.00 | | NIST Webbook |
| rinpol | 566.00 | | NIST Webbook |
| rinpol | 566.00 | | NIST Webbook |
| rinpol | 540.00 | | NIST Webbook |
| rinpol | 537.00 | | NIST Webbook |
| rinpol | 566.00 | | NIST Webbook |
| rinpol | 569.00 | | NIST Webbook |
| rinpol | 565.90 | | NIST Webbook |
| rinpol | 581.70 | | NIST Webbook |
| rinpol | 572.10 | | NIST Webbook |
| rinpol | 550.00 | | NIST Webbook |
| rinpol | 550.00 | | NIST Webbook |
| rinpol | 522.00 | | NIST Webbook |
| rinpol | 572.00 | | NIST Webbook |
| rinpol | 562.00 | | NIST Webbook |
| rinpol | 555.00 | | NIST Webbook |
| ripol | 773.00 | | NIST Webbook |
| sl | 233.55 | J/mol×K | NIST Webbook |
| tb | 325.70 | K | NIST Webbook |
| tb | 332.00 ± 4.00 | K | NIST Webbook |
| tb | 326.00 ± 2.00 | K | NIST Webbook |
| tb | 331.00 ± 3.00 | K | NIST Webbook |
| tb | 330.00 ± 5.00 | K | NIST Webbook |
| tb | 322.95 | K | KDB |
| tb | 331.70 | K | NIST Webbook |
| tb | 333.00 ± 1.38 | K | NIST Webbook |
| tb | 324.40 ± 0.70 | K | NIST Webbook |
| tb | 325.75 ± 0.20 | K | NIST Webbook |
| tb | 330.00 ± 3.00 | K | NIST Webbook |
| tb | 325.75 ± 0.30 | K | NIST Webbook |
| tb | 331.00 ± 2.00 | K | NIST Webbook |
| tb | 325.70 ± 0.20 | K | NIST Webbook |
| tb | 326.00 ± 3.00 | K | NIST Webbook |
| tb | 325.80 ± 0.30 | K | NIST Webbook |
| tb | 327.00 ± 4.00 | K | NIST Webbook |
| tb | 327.00 ± 2.00 | K | NIST Webbook |

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|---|---|---|---|
| tb | 325.70 | K | NIST Webbook |
| tb | 332.00 ± 6.00 | K | NIST Webbook |
| tb | 328.00 ± 3.00 | K | NIST Webbook |
| tc | 517.30 | K | NIST Webbook |
| tf | 142.61 ± 0.06 | K | NIST Webbook |
| tf | 142.61 ± 0.07 | K | NIST Webbook |
| tf | 142.63 | K | KDB |
| tf | 142.52 ± 0.20 | K | NIST Webbook |
| tf | 142.50 ± 0.30 | K | NIST Webbook |
| tt | 142.63 ± 0.10 | K | NIST Webbook |
| tt | 142.64 ± 0.06 | K | NIST Webbook |
| tt | 142.63 ± 0.08 | K | NIST Webbook |
| vc | 0.252 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 123.38 | J/mol×K | 428.44 | Joback Method |
| cpg | 129.68 | J/mol×K | 461.10 | Joback Method |
| cpg | 135.72 | J/mol×K | 493.76 | Joback Method |
| cpg | 102.84 | J/mol×K | 330.46 | Joback Method |
| cpg | 109.97 | J/mol×K | 363.12 | Joback Method |
| cpg | 116.82 | J/mol×K | 395.78 | Joback Method |
| cpg | 141.49 | J/mol×K | 526.42 | Joback Method |
| cpl | 145.35 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 5.73 | kJ/mol | 142.60 | NIST Webbook |
| hfust | 5.74 | kJ/mol | 142.60 | NIST Webbook |
| hfust | 0.05 | kJ/mol | 112.50 | NIST Webbook |
| hvapt | 31.90 | kJ/mol | 295.00 | NIST Webbook |
| hvapt | 27.91 | kJ/mol | 325.70 | NIST Webbook |
| hvapt | 27.91 | kJ/mol | 325.72 | NIST Webbook |
| sfust | 40.21 | J/mol×K | 142.60 | NIST Webbook |
| sfust | 0.46 | J/mol×K | 112.50 | NIST Webbook |
| svapt | 85.69 | J/mol×K | 325.72 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|

| Property code | pvap |
|---|---|
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.50317e+01 |
| Coeff. B | -3.08550e+03 |
| Coeff. C | -3.16970e+01 |
| Temperature range (K), min. | 240.97 |
| Temperature range (K), max. | 349.13 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 7.86655e+01 |
| Coeff. B | -6.03365e+03 |
| Coeff. C | -9.76729e+00 |
| Coeff. D | 9.34946e-06 |
| Temperature range (K), min. | 142.61 |
| Temperature range (K), max. | 517.00 |

# Sources

| | |
|---|---|
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Infinite dilution activity coefficient measurements by inert gas stripping method:** | https://www.doi.org/10.1016/j.fluid.2006.02.022 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Measurement of Henry s Law constant and infinite dilution activity coefficient of isopropyl mercaptan and isobutyl mercaptan in (methyldiethanolamine (1) + water (2)) with w1 = 0.25 and 0.50 at temperature of (298 to 348) K using inert gas stripping method:** | https://www.doi.org/10.1016/j.jct.2015.10.005 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1817.mol |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C75332&Units=SI |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1817 |

# Legend

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|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |

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|---|---|
| **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 |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **svapt:** | Entropy of vaporization at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |