# Benzene, (propylthio)-

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|---|---|
| **Other names:** | (1-Thiabutyl)benzene |
| | (Propylthio)benzene |
| | Fenyl-propylsulfid |
| | NSC 115079 |
| | Phenyl propyl sulfide |
| | Propyl phenyl sulfide |
| | Sulfide, phenyl propyl |
| | n-Propyl phenyl sulfide |
| **Inchi:** | InChI=1S/C9H12S/c1-2-8-10-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3 |
| **InchiKey:** | NWYDLOBJQIJDGH-UHFFFAOYSA-N |
| **Formula:** | C9H12S |
| **SMILES:** | CCCSc1ccccc1 |
| **Mol. weight [g/mol]:** | 152.26 |
| **CAS:** | 874-79-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 170.43 | kJ/mol | Joback Method |
| hf | 49.31 | kJ/mol | Joback Method |
| hfus | 17.24 | kJ/mol | Joback Method |
| hvap | 44.72 | kJ/mol | Joback Method |
| ie | 7.81 ± 0.03 | eV | NIST Webbook |
| log10ws | -3.05 | | Crippen Method |
| logp | 3.189 | | Crippen Method |
| mcvol | 130.260 | ml/mol | McGowan Method |
| pc | 3325.84 | kPa | Joback Method |
| rinpol | 1252.00 | | NIST Webbook |
| rinpol | 1252.00 | | NIST Webbook |
| rinpol | 1252.00 | | NIST Webbook |
| tb | 492.70 | K | NIST Webbook |
| tb | 491.00 ± 6.00 | K | NIST Webbook |
| tc | 731.34 | K | Joback Method |
| tf | 252.01 | K | Joback Method |
| vc | 0.485 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 265.38 | J/mol×K | 500.78 | Joback Method |
| cpg | 279.81 | J/mol×K | 539.21 | Joback Method |
| cpg | 293.33 | J/mol×K | 577.63 | Joback Method |
| cpg | 305.99 | J/mol×K | 616.06 | Joback Method |
| cpg | 317.80 | J/mol×K | 654.48 | Joback Method |
| cpg | 328.81 | J/mol×K | 692.91 | Joback Method |
| cpg | 339.05 | J/mol×K | 731.34 | Joback Method |
| hvapt | 44.30 | kJ/mol | 488.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.45598e+01 |
| Coeff. B | -4.14312e+03 |
| Coeff. C | -7.59500e+01 |
| Temperature range (K), min. | 366.24 |
| Temperature range (K), max. | 523.93 |

# Sources

**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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C874793&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# 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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |