# Sulfide, isopropyl phenyl

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|---|---|
| **Other names:** | (Isopropylthio)benzene |
| | Benzene, [(1-methylethyl)thio]- |
| | Isopropyl phenyl sulfide |
| | Phenyl isopropyl sulfide |
| **Inchi:** | InChI=1S/C9H12S/c1-8(2)10-9-6-4-3-5-7-9/h3-8H,1-2H3 |
| **InchiKey:** | SNOAHAUUBQMVGW-UHFFFAOYSA-N |
| **Formula:** | C9H12S |
| **SMILES:** | CC(C)Sc1ccccc1 |
| **Mol. weight [g/mol]:** | 152.26 |
| **CAS:** | 3019-20-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 167.99 | kJ/mol | Joback Method |
| hf | 44.03 | kJ/mol | Joback Method |
| hfus | 13.71 | kJ/mol | Joback Method |
| hvap | 44.33 | kJ/mol | Joback Method |
| ie | 7.90 | eV | NIST Webbook |
| ie | 8.46 | eV | NIST Webbook |
| log10ws | -3.16 | | Crippen Method |
| logp | 3.187 | | Crippen Method |
| mcvol | 130.260 | ml/mol | McGowan Method |
| pc | 3356.75 | kPa | Joback Method |
| rinpol | 1184.00 | | NIST Webbook |
| rinpol | 1184.00 | | NIST Webbook |
| tb | 500.34 | K | Joback Method |
| tc | 736.46 | K | Joback Method |
| tf | 237.01 | K | Joback Method |
| vc | 0.479 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 265.63 | J/mol×K | 500.34 | Joback Method |

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|---|---|---|---|---|
| cpg | 280.49 | J/mol×K | 539.69 | Joback Method |
| cpg | 294.39 | J/mol×K | 579.05 | Joback Method |
| cpg | 307.37 | J/mol×K | 618.40 | Joback Method |
| cpg | 319.45 | J/mol×K | 657.75 | Joback Method |
| cpg | 330.69 | J/mol×K | 697.10 | Joback Method |
| cpg | 341.10 | J/mol×K | 736.46 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.32442e+01 |
| Coeff. B | -3.65946e+03 |
| Coeff. C | -7.36700e+01 |
| Temperature range (K), min. | 356.11 |
| Temperature range (K), max. | 534.98 |

# Sources

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|---|---|
| **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=C3019203&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 |

# 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 |
| **ie:** | Ionization energy |

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