# Benzenethiol, o-isopropyl-

**Other names:** 2-Isopropylbenzenethiol
**Inchi:** InChI=1S/C9H12S/c1-7(2)8-5-3-4-6-9(8)10/h3-7,10H,1-2H3
**InchiKey:** QEDRUXIMTJVXFL-UHFFFAOYSA-N
**Formula:** C9H12S
**SMILES:** CC(C)c1ccccc1S
**Mol. weight [g/mol]:** 152.26
**CAS:** 6262-87-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 154.63 | kJ/mol | Joback Method |
| hf | 29.17 | kJ/mol | Joback Method |
| hfus | 13.24 | kJ/mol | Joback Method |
| hvap | 44.92 | kJ/mol | Joback Method |
| log10ws | -3.17 | | Crippen Method |
| logp | 3.099 | | Crippen Method |
| mcvol | 130.260 | ml/mol | McGowan Method |
| pc | 3484.76 | kPa | Joback Method |
| rinpol | 1237.40 | | NIST Webbook |
| tb | 493.20 | K | NIST Webbook |
| tc | 737.25 | K | Joback Method |
| tf | 251.59 | K | Joback Method |
| vc | 0.479 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 263.72 | J/mol×K | 499.40 | Joback Method |
| cpg | 278.10 | J/mol×K | 539.04 | Joback Method |
| cpg | 291.56 | J/mol×K | 578.68 | Joback Method |
| cpg | 304.15 | J/mol×K | 618.33 | Joback Method |
| cpg | 315.90 | J/mol×K | 657.97 | Joback Method |
| cpg | 326.85 | J/mol×K | 697.61 | Joback Method |
| cpg | 337.03 | J/mol×K | 737.25 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46434e+01 |
| Coeff. B | -4.15994e+03 |
| Coeff. C | -7.82460e+01 |
| Temperature range (K), min. | 368.02 |
| Temperature range (K), max. | 524.02 |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6262879&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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |
| **tb:** | Normal Boiling Point Temperature |

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |