# 4-Isopropylbenzenethiol, S-acetyl-

**Inchi:** InChI=1S/C11H14OS/c1-8(2)10-4-6-11(7-5-10)13-9(3)12/h4-8H,1-3H3
**InchiKey:** QMBWRQVNMADNBE-UHFFFAOYSA-N
**Formula:** C11H14OS
**SMILES:** CC(=O)Sc1ccc(C(C)C)cc1
**Mol. weight [g/mol]:** 194.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 46.28 | kJ/mol | Joback Method |
| hf | -121.30 | kJ/mol | Joback Method |
| hfus | 20.10 | kJ/mol | Joback Method |
| hvap | 56.19 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.449 | | Crippen Method |
| mcvol | 160.010 | ml/mol | McGowan Method |
| pc | 2859.68 | kPa | Joback Method |
| rinpol | 1530.70 | | NIST Webbook |
| tb | 604.95 | K | Joback Method |
| tc | 841.20 | K | Joback Method |
| tf | 322.00 | K | Joback Method |
| vc | 0.598 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 374.21 | J/mol×K | 604.95 | Joback Method |
| cpg | 389.04 | J/mol×K | 644.33 | Joback Method |
| cpg | 402.87 | J/mol×K | 683.70 | Joback Method |
| cpg | 415.73 | J/mol×K | 723.08 | Joback Method |
| cpg | 427.66 | J/mol×K | 762.45 | Joback Method |
| cpg | 438.67 | J/mol×K | 801.83 | Joback Method |
| cpg | 448.81 | J/mol×K | 841.20 | Joback Method |

# 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=U353047&Units=SI |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |