# 4-Isopropylbenzenethiol, S-methyl-

**Inchi:** InChI=1S/C10H14S/c1-8(2)9-4-6-10(11-3)7-5-9/h4-8H,1-3H3
**InchiKey:** IGKRCEMLHDKLEE-UHFFFAOYSA-N
**Formula:** C10H14S
**SMILES:** CSc1ccc(C(C)C)cc1
**Mol. weight [g/mol]:** 166.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 166.78 | kJ/mol | Joback Method |
| hf | 11.92 | kJ/mol | Joback Method |
| hfus | 15.92 | kJ/mol | Joback Method |
| hvap | 47.22 | kJ/mol | Joback Method |
| log10ws | -3.40 | | Crippen Method |
| logp | 3.532 | | Crippen Method |
| mcvol | 144.350 | ml/mol | McGowan Method |
| pc | 2963.34 | kPa | Joback Method |
| rinpol | 1371.70 | | NIST Webbook |
| rinpol | 1371.70 | | NIST Webbook |
| tb | 528.20 | K | Joback Method |
| tc | 761.14 | K | Joback Method |
| tf | 260.80 | K | Joback Method |
| vc | 0.535 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 310.01 | J/mol×K | 528.20 | Joback Method |
| cpg | 325.47 | J/mol×K | 567.02 | Joback Method |
| cpg | 339.98 | J/mol×K | 605.85 | Joback Method |
| cpg | 353.59 | J/mol×K | 644.67 | Joback Method |
| cpg | 366.32 | J/mol×K | 683.50 | Joback Method |
| cpg | 378.20 | J/mol×K | 722.32 | Joback Method |
| cpg | 389.25 | J/mol×K | 761.14 | Joback Method |

# Sources

| | |
|---|---|
| **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=U353048&Units=SI |
| **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 |
| **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 |

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