# 2-Mercaptophenol

**Other names:** Phenol, 2-mercapto-
o-mercaptophenol
**Inchi:** InChI=1S/C6H6OS/c7-5-3-1-2-4-6(5)8/h1-4,7-8H
**InchiKey:** VMKYTRPNOVFCGZ-UHFFFAOYSA-N
**Formula:** C6H6OS
**SMILES:** Oc1ccccc1S
**Mol. weight [g/mol]:** 126.18
**CAS:** 1121-24-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -13.18 | kJ/mol | Joback Method |
| hf | -69.47 | kJ/mol | Joback Method |
| hfus | 15.16 | kJ/mol | Joback Method |
| hvap | 50.98 | kJ/mol | Joback Method |
| log10ws | -1.53 | | Crippen Method |
| logp | 1.681 | | Crippen Method |
| mcvol | 93.860 | ml/mol | McGowan Method |
| pc | 6400.00 | kPa | Joback Method |
| tb | 506.84 | K | Joback Method |
| tc | 766.12 | K | Joback Method |
| tf | 331.98 | K | Joback Method |
| vc | 0.283 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 184.39 | J/mol×K | 506.84 | Joback Method |
| cpg | 193.79 | J/mol×K | 550.05 | Joback Method |
| cpg | 202.28 | J/mol×K | 593.27 | Joback Method |
| cpg | 209.98 | J/mol×K | 636.48 | Joback Method |
| cpg | 216.99 | J/mol×K | 679.69 | Joback Method |
| cpg | 223.42 | J/mol×K | 722.90 | Joback Method |
| cpg | 229.38 | J/mol×K | 766.12 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 489.70 | K | 100.00 | NIST Webbook |

# 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=C1121240&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |