# 2,3,5,6-Tetrafluorothiophenol

**Other names:** Benzenethiol, 2,3,5,6-tetrafluoro-
2,3,5,6-tetrafluorobenzenethiol
**Inchi:** InChI=1S/C6H2F4S/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H
**InchiKey:** IGOGJHYWSOZGAE-UHFFFAOYSA-N
**Formula:** C6H2F4S
**SMILES:** Fc1cc(F)c(F)c(S)c1F
**Mol. weight [g/mol]:** 182.14
**CAS:** 769-40-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -676.32 | kJ/mol | Joback Method |
| hf | -722.48 | kJ/mol | Joback Method |
| hfus | 20.14 | kJ/mol | Joback Method |
| hvap | 37.34 | kJ/mol | Joback Method |
| log10ws | -3.31 | | Crippen Method |
| logp | 2.532 | | Crippen Method |
| mcvol | 95.070 | ml/mol | McGowan Method |
| pc | 3722.56 | kPa | Joback Method |
| tb | 425.70 | K | NIST Webbook |
| tc | 641.82 | K | Joback Method |
| tf | 272.70 | K | Joback Method |
| vc | 0.390 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 177.91 | J/mol×K | 443.22 | Joback Method |
| cpg | 184.50 | J/mol×K | 476.32 | Joback Method |
| cpg | 190.79 | J/mol×K | 509.42 | Joback Method |
| cpg | 196.80 | J/mol×K | 542.52 | Joback Method |
| cpg | 202.52 | J/mol×K | 575.62 | Joback Method |
| cpg | 207.96 | J/mol×K | 608.72 | Joback Method |
| cpg | 213.12 | J/mol×K | 641.82 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C769404&Units=SI |
| **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 |

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