# 2,3,4,6-Tetrafluorophenyl isothiocyanate

**Inchi:** InChI=1S/C7HF4NS/c8-3-1-4(9)7(12-2-13)6(11)5(3)10/h1H
**InchiKey:** NRJUHOHJQHTIOM-UHFFFAOYSA-N
**Formula:** C7HF4NS
**SMILES:** Fc1cc(F)c(N=C=S)c(F)c1F
**Mol. weight [g/mol]:** 207.15
**CAS:** 84348-86-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -497.53 | kJ/mol | Joback Method |
| hvap | 43.27 | kJ/mol | Joback Method |
| log10ws | -3.72 | | Crippen Method |
| logp | 2.977 | | Crippen Method |
| mcvol | 110.540 | ml/mol | McGowan Method |
| pc | 3166.83 | kPa | Joback Method |
| tb | 549.19 | K | Joback Method |
| tc | 767.64 | K | 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=C84348867&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

**hf:** Enthalpy of formation 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 |