# 1-Chloro-2,3,5,6-tetrafluorobenzene

**Other names:** Benzene,3-chloro-1,2,4,5-tetrafluoro-
**Inchi:** InChI=1S/C6HClF4/c7-4-5(10)2(8)1-3(9)6(4)11/h1H
**InchiKey:** QLDHPPIOYFTGAJ-UHFFFAOYSA-N
**Formula:** C6HClF4
**SMILES:** Fc1cc(F)c(F)c(Cl)c1F
**Mol. weight [g/mol]:** 184.52
**CAS:** 1835-61-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -717.64 | kJ/mol | Joback Method |
| hf | -776.70 | kJ/mol | Joback Method |
| hfus | 20.30 | kJ/mol | Joback Method |
| hvap | 34.99 | kJ/mol | Joback Method |
| ie | 9.58 ± 0.02 | eV | NIST Webbook |
| log10ws | -3.48 | | Crippen Method |
| logp | 2.896 | | Crippen Method |
| mcvol | 90.960 | ml/mol | McGowan Method |
| pc | 3302.95 | kPa | Joback Method |
| tb | 417.79 | K | Joback Method |
| tc | 600.47 | K | Joback Method |
| tf | 266.16 | K | Joback Method |
| vc | 0.385 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 162.68 | J/mol×K | 417.79 | Joback Method |
| cpg | 168.45 | J/mol×K | 448.24 | Joback Method |
| cpg | 173.98 | J/mol×K | 478.68 | Joback Method |
| cpg | 179.27 | J/mol×K | 509.13 | Joback Method |
| cpg | 184.33 | J/mol×K | 539.58 | Joback Method |
| cpg | 189.17 | J/mol×K | 570.02 | Joback Method |
| cpg | 193.78 | J/mol×K | 600.47 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 399.00 | K | 98.50 | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1835616&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 |
| **ie:** | Ionization energy |
| **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 |

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