# 1,3-Dichloro-4-fluorobenzene

**Other names:** Benzene,2,4-dichloro-1-fluoro-
**Inchi:** InChI=1S/C6H3Cl2F/c7-4-1-2-6(9)5(8)3-4/h1-3H
**InchiKey:** BDJZCCWUSOZUQG-UHFFFAOYSA-N
**Formula:** C6H3Cl2F
**SMILES:** Fc1ccc(Cl)cc1Cl
**Mol. weight [g/mol]:** 164.99
**CAS:** 1435-48-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -125.88 | kJ/mol | Joback Method |
| hf | -181.17 | kJ/mol | Joback Method |
| hfus | 16.03 | kJ/mol | Joback Method |
| hvap | 40.50 | kJ/mol | Joback Method |
| log10ws | -3.17 | | Crippen Method |
| logp | 3.132 | | Crippen Method |
| mcvol | 97.890 | ml/mol | McGowan Method |
| pc | 3848.31 | kPa | Joback Method |
| tb | 447.45 | K | Joback Method |
| tc | 667.64 | K | Joback Method |
| tf | 269.27 | K | Joback Method |
| vc | 0.380 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 157.45 | J/mol×K | 447.45 | Joback Method |
| cpg | 164.82 | J/mol×K | 484.15 | Joback Method |
| cpg | 171.73 | J/mol×K | 520.85 | Joback Method |
| cpg | 178.19 | J/mol×K | 557.55 | Joback Method |
| cpg | 184.23 | J/mol×K | 594.25 | Joback Method |
| cpg | 189.87 | J/mol×K | 630.94 | Joback Method |
| cpg | 195.11 | J/mol×K | 667.64 | Joback Method |

# 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=C1435489&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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |