# 4-Fluoro-2-nitrophenol

**Other names:** Phenol, 4-fluoro-2-nitro-
**Inchi:** InChI=1S/C6H4FNO3/c7-4-1-2-6(9)5(3-4)8(10)11/h1-3,9H
**InchiKey:** ZHRLVDHMIJDWSS-UHFFFAOYSA-N
**Formula:** C6H4FNO3
**SMILES:** O=[N+]([O-])c1cc(F)ccc1O
**Mol. weight [g/mol]:** 157.10
**CAS:** 394-33-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -2731.10 | kJ/mol | NIST Webbook |
| gf | -211.46 | kJ/mol | Joback Method |
| hf | -326.29 | kJ/mol | Joback Method |
| hfus | 25.17 | kJ/mol | Joback Method |
| hvap | 60.68 | kJ/mol | Joback Method |
| log10ws | -2.00 | | Crippen Method |
| logp | 1.439 | | Crippen Method |
| mcvol | 96.700 | ml/mol | McGowan Method |
| pc | 5390.71 | kPa | Joback Method |
| tb | 600.07 | K | Joback Method |
| tc | 852.64 | K | Joback Method |
| tf | 452.24 | K | Joback Method |
| vc | 0.330 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 226.12 | J/mol×K | 600.07 | Joback Method |
| cpg | 234.01 | J/mol×K | 642.17 | Joback Method |
| cpg | 241.21 | J/mol×K | 684.26 | Joback Method |
| cpg | 247.81 | J/mol×K | 726.36 | Joback Method |
| cpg | 253.92 | J/mol×K | 768.45 | Joback Method |
| cpg | 259.63 | J/mol×K | 810.55 | Joback Method |
| cpg | 265.04 | J/mol×K | 852.64 | 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=C394332&Units=SI |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **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 |