# 4'-Fluoro-2'-nitroacetanilide

**Other names:** 4-Fluoro-2-nitroacetanilide
**Inchi:** InChI=1S/C8H7FN2O3/c1-5(12)10-7-3-2-6(9)4-8(7)11(13)14/h2-4H,1H3,(H,10,12)
**InchiKey:** UZBZEUCQENVPQB-UHFFFAOYSA-N
**Formula:** C8H7FN2O3
**SMILES:** CC(=O)Nc1ccc(F)cc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 198.15
**CAS:** 448-39-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3917.00 | kJ/mol | NIST Webbook |
| gf | -89.16 | kJ/mol | Joback Method |
| hf | -260.84 | kJ/mol | Joback Method |
| hfus | 30.88 | kJ/mol | Joback Method |
| hvap | 65.96 | kJ/mol | Joback Method |
| log10ws | -2.66 | | Crippen Method |
| logp | 1.692 | | Crippen Method |
| mcvol | 130.560 | ml/mol | McGowan Method |
| pc | 3708.97 | kPa | Joback Method |
| tb | 674.23 | K | Joback Method |
| tc | 912.12 | K | Joback Method |
| tf | 478.17 | K | Joback Method |
| vc | 0.516 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 326.64 | J/mol×K | 674.23 | Joback Method |
| cpg | 336.51 | J/mol×K | 713.88 | Joback Method |
| cpg | 345.61 | J/mol×K | 753.53 | Joback Method |
| cpg | 353.96 | J/mol×K | 793.18 | Joback Method |
| cpg | 361.59 | J/mol×K | 832.82 | Joback Method |
| cpg | 368.54 | J/mol×K | 872.47 | Joback Method |
| cpg | 374.85 | J/mol×K | 912.12 | 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=C448395&Units=SI |

# Legend

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|---|---|
| **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 |