# Acetamide, n-(4-fluorophenyl)-2-chloro-

**Inchi:** InChI=1S/C8H7ClFNO/c9-5-8(12)11-7-3-1-6(10)2-4-7/h1-4H,5H2,(H,11,12)
**InchiKey:** JDAWWCJBFPBHFL-UHFFFAOYSA-N
**Formula:** C8H7ClFNO
**SMILES:** O=C(CCl)Nc1ccc(F)cc1
**Mol. weight [g/mol]:** 187.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 24.10 | kJ/mol | Joback Method |
| ie | 8.62 | eV | Cheméo Relay (1.0) |
| log10ws | -2.20 | | Cheméo Relay (1.0) |
| logp | 2.003 | | Crippen Method |
| mcvol | 125.380 | ml/mol | McGowan Method |
| rinpol | 1417.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 266.25 | J/mol×K | 554.84 | Joback Method |
| cpg | 276.54 | J/mol×K | 591.02 | Joback Method |
| cpg | 286.15 | J/mol×K | 627.20 | Joback Method |
| cpg | 295.09 | J/mol×K | 663.38 | Joback Method |
| cpg | 303.40 | J/mol×K | 699.56 | Joback Method |
| cpg | 311.11 | J/mol×K | 735.74 | Joback Method |
| cpg | 318.24 | J/mol×K | 771.92 | Joback Method |

## Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307235&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |