# Benzophenone, 2-amino-2'-fluoro-5-nitro

**Other names:** 2-amino-5-nitro-2'-fluorobenzophenone
2-Amino-2'-fluoro-5-nitrobenzophenone
**Inchi:** InChI=1S/C13H9FN2O3/c14-11-4-2-1-3-9(11)13(17)10-7-8(16(18)19)5-6-12(10)15/h1-7H
**InchiKey:** ZTEHQPVGEHUXHI-UHFFFAOYSA-N
**Formula:** C13H9FN2O3
**SMILES:** Nc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1F
**Mol. weight [g/mol]:** 260.22
**CAS:** 344-80-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 32.78 | kJ/mol | Joback Method |
| hf | -158.66 | kJ/mol | Joback Method |
| hfus | 37.58 | kJ/mol | Joback Method |
| hvap | 84.23 | kJ/mol | Joback Method |
| log10ws | -4.05 | | Crippen Method |
| logp | 2.547 | | Crippen Method |
| mcvol | 177.250 | ml/mol | McGowan Method |
| pc | 3220.98 | kPa | Joback Method |
| rinpol | 2401.00 | | NIST Webbook |
| rinpol | 2363.00 | | NIST Webbook |
| rinpol | 2335.00 | | NIST Webbook |
| rinpol | 2401.00 | | NIST Webbook |
| rinpol | 2344.00 | | NIST Webbook |
| rinpol | 2335.00 | | NIST Webbook |
| rinpol | 2363.00 | | NIST Webbook |
| tb | 842.65 | K | Joback Method |
| tc | 1107.48 | K | Joback Method |
| tf | 604.06 | K | Joback Method |
| vc | 0.682 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 490.76 | J/mol×K | 842.65 | Joback Method |
| cpg | 500.87 | J/mol×K | 886.79 | Joback Method |
| cpg | 509.92 | J/mol×K | 930.93 | Joback Method |
| cpg | 517.98 | J/mol×K | 975.06 | Joback Method |
| cpg | 525.13 | J/mol×K | 1019.20 | Joback Method |
| cpg | 531.45 | J/mol×K | 1063.34 | Joback Method |
| cpg | 537.01 | J/mol×K | 1107.48 | Joback Method |

# Sources

| | |
|---|---|
| **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=C344809&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |