# 2,5-Diamino-2'-fluorobenzophenone

**Other names:** 2,5-Diamino-2'-fluor-benzophenone
Benzophenone, 2,5-diamino-2'-fluoro
**Inchi:** InChI=1S/C13H11FN2O/c14-11-4-2-1-3-9(11)13(17)10-7-8(15)5-6-12(10)16/h1-7H,15-16
**InchiKey:** OKCCYEPCUCOYDR-UHFFFAOYSA-N
**Formula:** C13H11FN2O
**SMILES:** Nc1ccc(N)c(C(=O)c2ccccc2F)c1
**Mol. weight [g/mol]:** 230.24
**CAS:** 67739-74-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 63.68 | kJ/mol | Joback Method |
| hf | -114.11 | kJ/mol | Joback Method |
| hfus | 31.41 | kJ/mol | Joback Method |
| hvap | 78.28 | kJ/mol | Joback Method |
| log10ws | -3.03 | | Crippen Method |
| logp | 2.221 | | Crippen Method |
| mcvol | 169.810 | ml/mol | McGowan Method |
| pc | 3392.03 | kPa | Joback Method |
| rinpol | 2188.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2188.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| tb | 763.34 | K | Joback Method |
| tc | 1016.00 | K | Joback Method |
| tf | 543.71 | K | Joback Method |
| vc | 0.629 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 458.57 | J/mol×K | 763.34 | Joback Method |
| cpg | 470.29 | J/mol×K | 805.45 | Joback Method |
| cpg | 480.97 | J/mol×K | 847.56 | Joback Method |

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|---|---|---|---|---|
| cpg | 490.67 | J/mol×K | 889.67 | Joback Method |
| cpg | 499.45 | J/mol×K | 931.78 | Joback Method |
| cpg | 507.37 | J/mol×K | 973.89 | Joback Method |
| cpg | 514.48 | J/mol×K | 1016.00 | Joback Method |

# Sources

| | |
|---|---|
| **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=C67739746&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |