# 2,3,4,5,6-Pentafluoro-N-(4-fluorophenyl)benzamid

**Other names:** Benzamide, N-(4-fluorophenyl)-2,3,4,5,6-pentafluoro-
**Inchi:** InChI=1S/C13H5F6NO/c14-5-1-3-6(4-2-5)20-13(21)7-8(15)10(17)12(19)11(18)9(7)16/h1-
**InchiKey:** NXSQZVGPHXRXGT-UHFFFAOYSA-N
**Formula:** C13H5F6NO
**SMILES:** O=C(Nc1ccc(F)cc1)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 305.18
**CAS:** 209109-65-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -982.77 | kJ/mol | Joback Method |
| hf | -1143.18 | kJ/mol | Joback Method |
| hfus | 40.35 | kJ/mol | Joback Method |
| hvap | 61.34 | kJ/mol | Joback Method |
| log10ws | -5.44 | | Crippen Method |
| logp | 3.773 | | Crippen Method |
| mcvol | 168.680 | ml/mol | McGowan Method |
| pc | 2293.71 | kPa | Joback Method |
| rinpol | 1716.00 | | NIST Webbook |
| tb | 679.74 | K | Joback Method |
| tc | 875.59 | K | Joback Method |
| tf | 470.36 | K | Joback Method |
| vc | 0.697 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 431.93 | J/mol×K | 679.74 | Joback Method |
| cpg | 441.80 | J/mol×K | 712.38 | Joback Method |
| cpg | 451.04 | J/mol×K | 745.02 | Joback Method |
| cpg | 459.66 | J/mol×K | 777.66 | Joback Method |
| cpg | 467.66 | J/mol×K | 810.30 | Joback Method |
| cpg | 475.08 | J/mol×K | 842.95 | Joback Method |
| cpg | 481.93 | J/mol×K | 875.59 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C209109659&Units=SI |
| **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 |

# Legend

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