# 4-Cyanobenzophenone

**Other names:** Benzonitrile, 4-benzoyl-
4-Cyano-benzophenon
4-benzoylbenzonitrile
**Inchi:** InChI=1S/C14H9NO/c15-10-11-6-8-13(9-7-11)14(16)12-4-2-1-3-5-12/h1-9H
**InchiKey:** YSZWJJANSNFQMM-UHFFFAOYSA-N
**Formula:** C14H9NO
**SMILES:** N#Cc1ccc(C(=O)c2ccccc2)cc1
**Mol. weight [g/mol]:** 207.23
**CAS:** 1503-49-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 1.26 ± 0.09 | eV | NIST Webbook |
| gf | 286.45 | kJ/mol | Joback Method |
| hf | 181.60 | kJ/mol | Joback Method |
| hfus | 22.81 | kJ/mol | Joback Method |
| hvap | 69.20 | kJ/mol | Joback Method |
| log10ws | -3.78 | | Crippen Method |
| logp | 2.789 | | Crippen Method |
| mcvol | 163.550 | ml/mol | McGowan Method |
| pc | 2838.39 | kPa | Joback Method |
| tb | 734.01 | K | Joback Method |
| tc | 992.70 | K | Joback Method |
| tf | 427.82 | K | Joback Method |
| vc | 0.635 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 409.60 | J/mol×K | 734.01 | Joback Method |
| cpg | 421.47 | J/mol×K | 777.12 | Joback Method |
| cpg | 432.23 | J/mol×K | 820.24 | Joback Method |
| cpg | 441.97 | J/mol×K | 863.35 | Joback Method |
| cpg | 450.77 | J/mol×K | 906.47 | Joback Method |

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|---|---|---|---|---|
| cpg | 458.71 | J/mol×K | 949.58 | Joback Method |
| cpg | 465.87 | J/mol×K | 992.70 | 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=C1503497&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **ea:** | Electron affinity |
| **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 |