# 2,5-DIAMINOBENZOPHENONE

**Other names:** (2,5-Diaminophenyl)(phenyl)methanone
Benzophenone, 2,5-diamino
Methanone, (2,5-diaminophenyl)phenyl-
**Inchi:** InChI=1S/C13H12N2O/c14-10-6-7-12(15)11(8-10)13(16)9-4-2-1-3-5-9/h1-8H,14-15H2
**InchiKey:** WJWKTVHKQDEXEQ-UHFFFAOYSA-N
**Formula:** C13H12N2O
**SMILES:** Nc1ccc(N)c(C(=O)c2ccccc2)c1
**Mol. weight [g/mol]:** 212.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 45.84 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 28.72 | kJ/mol | Joback Method |
| hvap | 103.88 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.70 | eV | Cheméo Relay (1.0) |
| log10ws | -3.00 | | Cheméo Relay (1.0) |
| logp | 2.082 | | Crippen Method |
| mcvol | 168.040 | ml/mol | McGowan Method |
| pc | 3642.13 | kPa | Joback Method |
| rinpol | 2198.00 | | NIST Webbook |
| tb | 651.64 | K | Cheméo Relay (1.0) |
| tc | 957.37 | K | Cheméo Relay (1.0) |
| tf | 416.22 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 452.40 | J/mol×K | 759.09 | Joback Method |
| cpg | 464.90 | J/mol×K | 803.03 | Joback Method |
| cpg | 476.24 | J/mol×K | 846.97 | Joback Method |
| cpg | 486.50 | J/mol×K | 890.91 | Joback Method |
| cpg | 495.77 | J/mol×K | 934.85 | Joback Method |
| cpg | 504.11 | J/mol×K | 978.79 | Joback Method |
| cpg | 511.62 | J/mol×K | 1022.73 | Joback Method |

# Sources

| | |
|---|---|
| **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=C18330944&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |