# Acetophenone, 2-phenyl-2-(4-chlorophenylamino)

**Inchi:** InChI=1S/C20H16ClNO/c21-17-11-13-18(14-12-17)22-19(15-7-3-1-4-8-15)20(23)16-9-5-

**InchiKey:** OKXHEPYTJQIFQB-UHFFFAOYSA-N

**Formula:** C20H16ClNO

**SMILES:** O=C(c1ccccc1)C(Nc1ccc(Cl)cc1)c1ccccc1

**Mol. weight [g/mol]:** 321.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 391.22 | kJ/mol | Joback Method |
| hf | 161.86 | kJ/mol | Joback Method |
| hfus | 36.66 | kJ/mol | Joback Method |
| hvap | 84.78 | kJ/mol | Joback Method |
| log10ws | -6.13 | | Crippen Method |
| logp | 5.376 | | Crippen Method |
| mcvol | 245.170 | ml/mol | McGowan Method |
| pc | 2239.76 | kPa | Joback Method |
| rinpol | 2669.00 | | NIST Webbook |
| rinpol | 2669.00 | | NIST Webbook |
| tb | 883.05 | K | Joback Method |
| tc | 1146.66 | K | Joback Method |
| tf | 524.45 | K | Joback Method |
| vc | 0.915 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 694.31 | J/mol×K | 883.05 | Joback Method |
| cpg | 707.76 | J/mol×K | 926.98 | Joback Method |
| cpg | 719.88 | J/mol×K | 970.92 | Joback Method |
| cpg | 730.83 | J/mol×K | 1014.85 | Joback Method |
| cpg | 740.75 | J/mol×K | 1058.79 | Joback Method |
| cpg | 749.79 | J/mol×K | 1102.72 | Joback Method |
| cpg | 758.09 | J/mol×K | 1146.66 | 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=R121118&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 |