# Benzamide, N-(3-chlorophenyl)-4-nitro-

**Inchi:** InChI=1S/C13H9ClN2O3/c14-10-2-1-3-11(8-10)15-13(17)9-4-6-12(7-5-9)16(18)19/h1-8H
**InchiKey:** KVVNRXNSICWUSG-UHFFFAOYSA-N
**Formula:** C13H9ClN2O3
**SMILES:** O=C(Nc1cccc(Cl)c1)c1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 276.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 248.23 | kJ/mol | Joback Method |
| hf | 52.86 | kJ/mol | Joback Method |
| hfus | 38.99 | kJ/mol | Joback Method |
| hvap | 84.57 | kJ/mol | Joback Method |
| log10ws | -4.78 | | Crippen Method |
| logp | 3.500 | | Crippen Method |
| mcvol | 187.720 | ml/mol | McGowan Method |
| pc | 3145.56 | kPa | Joback Method |
| rinpol | 2602.00 | | NIST Webbook |
| tb | 853.47 | K | Joback Method |
| tc | 1122.75 | K | Joback Method |
| tf | 590.27 | K | Joback Method |
| vc | 0.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 498.61 | J/mol×K | 853.47 | Joback Method |
| cpg | 508.57 | J/mol×K | 898.35 | Joback Method |
| cpg | 517.46 | J/mol×K | 943.23 | Joback Method |
| cpg | 525.35 | J/mol×K | 988.11 | Joback Method |
| cpg | 532.35 | J/mol×K | 1032.99 | Joback Method |
| cpg | 538.56 | J/mol×K | 1077.87 | Joback Method |
| cpg | 544.05 | J/mol×K | 1122.75 | Joback Method |

# Sources

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|---|---|
| **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=U307352&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |