# 2-Amino-4-chlorobenzoic acid

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|---|---|
| **Other names:** | 4-Chloro anthranilic acid |
| | 4-chloroanthranil acid |
| | 4-chloroanthranilic acid |
| | Anthranilic acid, 4-chloro- |
| | Benzoic acid, 2-amino-4-chloro- |
| **Inchi:** | InChI=1S/C7H6ClNO2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,9H2,(H,10,11) |
| **InchiKey:** | JYYLQSCZISREGY-UHFFFAOYSA-N |
| **Formula:** | C7H6ClNO2 |
| **SMILES:** | Nc1cc(Cl)ccc1C(=O)O |
| **Mol. weight [g/mol]:** | 171.58 |
| **CAS:** | 89-77-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -110.01 | kJ/mol | Joback Method |
| hf | -220.98 | kJ/mol | Joback Method |
| hfus | 22.23 | kJ/mol | Joback Method |
| hvap | 73.23 | kJ/mol | Joback Method |
| log10ws | -1.85 | | Crippen Method |
| logp | 1.620 | | Crippen Method |
| mcvol | 115.390 | ml/mol | McGowan Method |
| pc | 5001.51 | kPa | Joback Method |
| tb | 652.21 | K | Joback Method |
| tc | 875.53 | K | Joback Method |
| tf | 507.50 | K | Solubility determination and thermodynamic modelling for 2-amino-4-chlorobenzoic acid in eleven organic solvents from T = (278.15 to 313.15) K and mixing properties of solutions |
| vc | 0.422 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 257.90 | J/mol×K | 652.21 | Joback Method |
| cpg | 265.20 | J/mol×K | 689.43 | Joback Method |
| cpg | 271.97 | J/mol×K | 726.65 | Joback Method |
| cpg | 278.24 | J/mol×K | 763.87 | Joback Method |
| cpg | 284.04 | J/mol×K | 801.09 | Joback Method |
| cpg | 289.38 | J/mol×K | 838.31 | Joback Method |
| cpg | 294.28 | J/mol×K | 875.53 | Joback Method |

# Sources

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| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Solubility determination and thermodynamic modelling for 2-amino-4-chlorobenzoic acid in eleven organic solvents from T = (278.15 to 318.15) K and mixing properties of solutions:** | https://www.doi.org/10.1016/j.jct.2016.11.019 |
| **Solubility Measurement and Modeling of 2-Amino-4,6-dichloropyrimidine in Eleven Organic Solvents from 278.15 to 318.15 K and Thermodynamic Dissolution Properties in Ethanol + Solvent Mixtures:** | https://www.doi.org/10.1021/acs.jced.8b00292 |
| **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=C89770&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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