

Benzoic acid, 4-amino-2-chloro-

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| Other names: | o-Chloro-p-aminobenzoic acid 2-Chloro-p-aminobenzoic acid 2-Chloro-4-aminobenzoic acid 4-Amino-2-chlorobenzoic acid USAF nb-1 |
| Inchi: | InChI=1S/C7H6ClNO2/c8-6-3-4(9)1-2-5(6)7(10)11/h1-3H,9H2,(H,10,11) |
| InchiKey: | MBDUKNCPOPJRJQ-UHFFFAOYSA-N |
| Formula: | C7H6ClNO2 |
| SMILES: | <chem>Nc1ccc(C(=O)O)c(Cl)c1</chem> |
| Mol. weight [g/mol]: | 171.58 |
| CAS: | 2457-76-3 |

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 |
| mccvol | 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 | 444.04 | K | Joback Method |
| vc | 0.422 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

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

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|-----|--------|---------|--------|---------------|
| 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

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2457763&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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