# anthranilamide

**Inchi:** InChI=1S/C7H8N2O/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,8H2,(H2,9,10)
**InchiKey:** PXBFMLJZNCDSMP-UHFFFAOYSA-N
**Formula:** C7H8N2O
**SMILES:** NC(=O)c1ccccc1N
**Mol. weight [g/mol]:** 136.15

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 114.82 | kJ/mol | Joback Method |
| hf | -7.75 | kJ/mol | Joback Method |
| hfus | 21.90 | kJ/mol | Solubility Measurement and Phase Equilibrium Modeling of 2-Aminobenzamide in 15 Pure Solvents |
| hfus | 20.90 | kJ/mol | Experimental and computational thermodynamic study of ortho- meta- and para-aminobenzamide |
| hvap | 62.14 | kJ/mol | Joback Method |
| log10ws | -1.28 | | Crippen Method |
| logp | 0.368 | | Crippen Method |
| mcvol | 107.260 | ml/mol | McGowan Method |
| pc | 5123.98 | kPa | Joback Method |
| tb | 590.15 | K | Joback Method |
| tc | 837.19 | K | Joback Method |
| tf | 424.04 | K | Joback Method |
| tt | 384.40 | K | Experimental and computational thermodynamic study of ortho- meta- and para-aminobenzamide |
| tt | 383.65 | K | Solubility Measurement and Phase Equilibrium Modeling of 2-Aminobenzamide in 15 Pure Solvents |
| vc | 0.384 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 248.85 | J/mol×K | 590.15 | Joback Method |
| cpg | 259.00 | J/mol×K | 631.32 | Joback Method |
| cpg | 268.39 | J/mol×K | 672.50 | Joback Method |
| cpg | 277.04 | J/mol×K | 713.67 | Joback Method |
| cpg | 284.99 | J/mol×K | 754.84 | Joback Method |
| cpg | 292.28 | J/mol×K | 796.02 | Joback Method |
| cpg | 298.94 | J/mol×K | 837.19 | Joback Method |
| psub | 1.50e-04 | kPa | 339.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.21e-04 | kPa | 337.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.52e-04 | kPa | 339.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.87e-04 | kPa | 341.10 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 2.36e-04 | kPa | 343.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 2.98e-04 | kPa | 345.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 3.59e-04 | kPa | 347.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |

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|---|---|---|---|---|
| psub | 4.41e-04 | kPa | 349.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 5.45e-04 | kPa | 351.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 6.67e-04 | kPa | 353.12 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 8.20e-04 | kPa | 355.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.93e-04 | kPa | 357.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.60e-05 | kPa | 335.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.21e-04 | kPa | 337.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.50e-05 | kPa | 335.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.90e-04 | kPa | 341.10 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 2.37e-04 | kPa | 343.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |

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|---|---|---|---|---|
| psub | 2.90e-04 | kPa | 345.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 3.59e-04 | kPa | 347.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 4.45e-04 | kPa | 349.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 5.39e-04 | kPa | 351.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 6.67e-04 | kPa | 353.12 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 8.26e-04 | kPa | 355.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.94e-04 | kPa | 357.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.50e-05 | kPa | 335.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.20e-04 | kPa | 337.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 1.49e-04 | kPa | 339.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |

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|---|---|---|---|---|
| psub | 1.88e-04 | kPa | 341.10 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 2.32e-04 | kPa | 343.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 2.85e-04 | kPa | 345.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 3.57e-04 | kPa | 347.11 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 4.35e-04 | kPa | 349.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 5.30e-04 | kPa | 351.17 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 6.63e-04 | kPa | 353.12 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 8.06e-04 | kPa | 355.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |
| psub | 9.93e-04 | kPa | 357.16 | Experimental and computational thermodynamic study of ortho-meta- and para-aminobenzamide |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Experimental and computational thermodynamic study of ortho- meta- and para-aminobenzamide:** | https://www.doi.org/10.1016/j.jct.2012.12.006 |
| **Solubility Measurement and Phase Equilibrium Modeling of 2-Aminobenzamide in 15 Pure Solvents:** | https://www.doi.org/10.1021/acs.jced.9b00350 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **psub:** | Sublimation pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |