# 2-acetamidobenzoic acid

**Other names:** N-acetylanthranilic acid
o-acetamidobenzoic acid
**Inchi:** InChI=1S/C9H9NO3/c1-6(11)10-8-5-3-2-4-7(8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
**InchiKey:** QSACCXVHEVWNMX-UHFFFAOYSA-N
**Formula:** C9H9NO3
**SMILES:** CC(=O)Nc1ccccc1C(=O)O
**Mol. weight [g/mol]:** 179.18

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -177.59 | kJ/mol | Joback Method |
| hf | -327.95 | kJ/mol | Joback Method |
| hfus | 29.32 | kJ/mol | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| hfus | 49.40 | kJ/mol | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| hvap | 75.17 | kJ/mol | Joback Method |
| log10ws | -1.73 | | Crippen Method |
| logp | 1.343 | | Crippen Method |
| mcvol | 132.900 | ml/mol | McGowan Method |
| pc | 4244.08 | kPa | Joback Method |
| tb | 687.07 | K | Joback Method |
| tc | 898.02 | K | Joback Method |
| tf | 458.40 | K | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| tf | 455.11 | K | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| vc | 0.497 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 380.73 | J/mol×K | 898.02 | Joback Method |
| cpg | 374.62 | J/mol×K | 862.86 | Joback Method |
| cpg | 367.97 | J/mol×K | 827.70 | Joback Method |
| cpg | 360.77 | J/mol×K | 792.54 | Joback Method |
| cpg | 352.97 | J/mol×K | 757.39 | Joback Method |
| cpg | 344.57 | J/mol×K | 722.23 | Joback Method |
| cpg | 335.53 | J/mol×K | 687.07 | Joback Method |
| psub | 3.73e-04 | kPa | 381.29 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 7.80e-04 | kPa | 387.26 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 8.40e-04 | kPa | 389.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 8.30e-05 | kPa | 367.17 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 1.09e-04 | kPa | 369.28 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |

| | | | | |
|---|---|---|---|---|
| psub | 1.60e-04 | kPa | 373.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 2.07e-04 | kPa | 375.26 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 2.48e-04 | kPa | 377.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 3.05e-04 | kPa | 379.19 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 3.85e-04 | kPa | 381.29 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 5.77e-04 | kPa | 385.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 6.97e-04 | kPa | 387.26 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |

| | | | | | |
|---|---|---|---|---|---|
| psub | 8.29e-04 | kPa | 389.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 8.30e-05 | kPa | 367.17 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 1.08e-04 | kPa | 369.28 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 1.28e-04 | kPa | 371.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 2.10e-04 | kPa | 375.26 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 2.55e-04 | kPa | 377.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 3.03e-04 | kPa | 379.19 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |

| | | | | | |
|---|---|---|---|---|---|
| psub | 5.74e-04 | kPa | 385.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 5.61e-04 | kPa | 385.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 7.11e-04 | kPa | 387.26 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 8.40e-04 | kPa | 389.15 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids | |
| psub | 1.66e-05 | kPa | 344.70 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures | |
| psub | 3.37e-05 | kPa | 351.30 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures | |
| psub | 5.58e-05 | kPa | 357.30 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures | |

| | | | | |
|---|---|---|---|---|
| psub | 1.11e-04 | kPa | 363.50 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 1.16e-04 | kPa | 363.80 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 1.38e-04 | kPa | 366.20 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 2.35e-04 | kPa | 369.70 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 2.43e-04 | kPa | 371.00 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 2.89e-04 | kPa | 373.50 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 5.55e-04 | kPa | 377.40 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |

| | | | | |
|---|---|---|---|---|
| psub | 5.71e-04 | kPa | 380.00 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 9.48e-04 | kPa | 383.80 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 1.17e-03 | kPa | 387.20 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 1.52e-03 | kPa | 390.40 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 1.98e-03 | kPa | 393.50 | Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures |
| psub | 4.38e-04 | kPa | 383.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 3.78e-04 | kPa | 381.29 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |

| | | | | |
|---|---|---|---|---|
| psub | 3.08e-04 | kPa | 379.19 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 2.58e-04 | kPa | 377.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 1.63e-04 | kPa | 373.16 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 1.06e-04 | kPa | 369.28 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |
| psub | 8.30e-05 | kPa | 367.17 | Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids:** | https://www.doi.org/10.1016/j.jct.2015.02.010 |
| **Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures:** | https://www.doi.org/10.1016/j.tca.2014.03.019 |
| **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 |
| **vc:** | Critical Volume |