# Benzoic acid, 4-amino-3-hydroxy-, methyl ester

**Inchi:** InChI=1S/C8H9NO3/c1-12-8(11)5-2-3-6(9)7(10)4-5/h2-4,10H,9H2,1H3
**InchiKey:** OCZXDVNSNDITBS-UHFFFAOYSA-N
**Formula:** C8H9NO3
**SMILES:** COC(=O)c1ccc(N)c(O)c1
**Mol. weight [g/mol]:** 167.16
**CAS:** 63435-16-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -202.83 | kJ/mol | Joback Method |
| hf | -371.71 | kJ/mol | Joback Method |
| hfus | 23.89 | kJ/mol | Joback Method |
| hvap | 69.15 | kJ/mol | Joback Method |
| log10ws | -0.90 | | Crippen Method |
| logp | 0.761 | | Crippen Method |
| mcvol | 123.110 | ml/mol | McGowan Method |
| pc | 4973.33 | kPa | Joback Method |
| tb | 643.54 | K | Joback Method |
| tc | 883.84 | K | Joback Method |
| tf | 486.00 | K | Joback Method |
| vc | 0.395 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 307.53 | J/mol×K | 643.54 | Joback Method |
| cpg | 317.32 | J/mol×K | 683.59 | Joback Method |
| cpg | 326.45 | J/mol×K | 723.64 | Joback Method |
| cpg | 334.97 | J/mol×K | 763.69 | Joback Method |
| cpg | 342.95 | J/mol×K | 803.74 | Joback Method |
| cpg | 350.46 | J/mol×K | 843.79 | Joback Method |
| cpg | 357.56 | J/mol×K | 883.84 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C63435165&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |