# Benzoic acid, 2-amino-, propyl ester

**Other names:** propyl anthranilate
propyl 2-aminobenzoate
**Inchi:** InChI=1S/C10H13NO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7,11H2,1H3
**InchiKey:** QYGHESHPPSSONP-UHFFFAOYSA-N
**Formula:** C10H13NO2
**SMILES:** CCCOC(=O)c1ccccc1N
**Mol. weight [g/mol]:** 179.22
**CAS:** 30954-98-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -31.37 | kJ/mol | Joback Method |
| hf | -235.68 | kJ/mol | Joback Method |
| hfus | 23.29 | kJ/mol | Joback Method |
| hvap | 60.59 | kJ/mol | Joback Method |
| log10ws | -2.19 | | Crippen Method |
| logp | 1.836 | | Crippen Method |
| mcvol | 145.420 | ml/mol | McGowan Method |
| pc | 3231.98 | kPa | Joback Method |
| rinpol | 1500.00 | | NIST Webbook |
| rinpol | 1538.00 | | NIST Webbook |
| rinpol | 1500.00 | | NIST Webbook |
| rinpol | 1538.00 | | NIST Webbook |
| ripol | 2320.00 | | NIST Webbook |
| tb | 608.68 | K | Joback Method |
| tc | 830.79 | K | Joback Method |
| tf | 396.82 | K | Joback Method |
| vc | 0.540 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 357.09 | J/mol×K | 608.68 | Joback Method |
| cpg | 370.13 | J/mol×K | 645.70 | Joback Method |

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|---|---|---|---|---|
| cpg | 382.38 | J/mol×K | 682.72 | Joback Method |
| cpg | 393.85 | J/mol×K | 719.74 | Joback Method |
| cpg | 404.56 | J/mol×K | 756.76 | Joback Method |
| cpg | 414.52 | J/mol×K | 793.78 | Joback Method |
| cpg | 423.76 | J/mol×K | 830.79 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C30954984&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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |