# Methyl anthranilate

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|---|---|
| **Other names:** | 2-(Methoxycarbonyl)aniline |
| | 2-Aminobenzoic acid methyl ester |
| | 2-Carbomethoxyaniline |
| | 2-aminobenzoic acid, methyl ester |
| | Benzoic acid, 2-amino-, methyl ester |
| | Methyl anthranylate |
| | Methyl ester of o-Aminobenzoic acid |
| | Methyl o-aminobenzoate |
| | Methylester kyseliny anthranilove |
| | NSC 3109 |
| | Neroli oil, artifical |
| | Neroli oil, artificial |
| | Nevoli oil |
| | anthranilic acid, methyl ester |
| | methyl 2-aminobenzoate |
| | o-Amino methyl benzoate |
| | o-Aminobenzoic acid, methyl ester |
| | o-Carbomethoxyaniline |
| **Inchi:** | InChI=1S/C8H9NO2/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5H,9H2,1H3 |
| **InchiKey:** | VAMXMNNIEUEQDV-UHFFFAOYSA-N |
| **Formula:** | C8H9NO2 |
| **SMILES:** | COC(=O)c1ccccc1N |
| **Mol. weight [g/mol]:** | 151.16 |
| **CAS:** | 134-20-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -48.21 | kJ/mol | Joback Method |
| hf | -194.40 | kJ/mol | Joback Method |
| hfus | 17.90 | kJ/mol | Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids |
| hvap | 56.14 | kJ/mol | Joback Method |
| log10ws | -1.35 | | Crippen Method |
| logp | 1.055 | | Crippen Method |
| mcvol | 117.240 | ml/mol | McGowan Method |

| pc | 4072.51 | kPa | Joback Method |
|---|---|---|---|
| rinpol | 1329.00 | | NIST Webbook |
| rinpol | 1343.00 | | NIST Webbook |
| rinpol | 1309.00 | | NIST Webbook |
| rinpol | 1332.00 | | NIST Webbook |
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| ripol | 2198.00 | | NIST Webbook |
| ripol | 2197.00 | | NIST Webbook |
| ripol | 2244.00 | | NIST Webbook |
| ripol | 2206.00 | | NIST Webbook |
| ripol | 2236.00 | | NIST Webbook |
| tb | 529.20 | K | NIST Webbook |
| tc | 793.64 | K | Joback Method |
| tf | 297.50 ± 0.50 | K | NIST Webbook |
| tf | 298.65 ± 1.00 | K | NIST Webbook |
| tf | 297.60 ± 0.02 | K | NIST Webbook |
| vc | 0.428 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 305.72 | J/mol×K | 716.73 | Joback Method |
| cpg | 314.25 | J/mol×K | 755.19 | Joback Method |
| cpg | 264.93 | J/mol×K | 562.92 | Joback Method |
| cpg | 276.15 | J/mol×K | 601.37 | Joback Method |
| cpg | 286.68 | J/mol×K | 639.83 | Joback Method |
| cpg | 296.53 | J/mol×K | 678.28 | Joback Method |
| cpg | 322.15 | J/mol×K | 793.64 | Joback Method |
| hsubt | 78.40 | kJ/mol | 292.50 | NIST Webbook |
| hvapt | 62.30 | kJ/mol | 316.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 406.60 | K | 2.00 | NIST Webbook |

# Sources

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|---|---|
| **Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids:** | https://www.doi.org/10.1016/j.jct.2012.04.006 |
| **Ternary and Quaternary Liquid Liquid Equilibria for Systems of Water + Methanol + Methylanthranilate + Toluene at Different Temperatures:** | https://www.doi.org/10.1021/je300585v |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C134203&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Liquid-liquid equilibria for systems of water + methanol + methyl anthranilate at several temperatures:** | https://www.doi.org/10.1016/j.fluid.2011.07.008 |

# 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 |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |