# Benzoic acid, 2-(methylamino)-, methyl ester

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|---|---|
| **Other names:** | Anthranilic acid, N-methyl-, methyl ester |
| | Methyl methanthranilate |
| | Methyl methylanthranilate |
| | Methyl o-(methylamino)benzoate |
| | Methyl N-methyl-o-anthranilate |
| | Methyl N-methylanthranilate |
| | N-Methylanthranilic acid, methyl ester |
| | Methyl-2-(N-methylamino)benzoate |
| | 2-Methylaminobenzoic acid methyl ester |
| | Dimethyl anthranilate |
| | Methyl 2-methylaminobenzoate |
| | Methyl m-methylanthranilate |
| | Methyl methylaminobenzoate |
| | N-Methyl methyl anthranilate |
| | 2-Methylaminomethyl benzoate |
| | Benzoic acid, o-(methylamino)-, methyl ester |
| | Me N-methylanthranilate |
| | Me N-methylanthranylate |
| | Methyl benzoate, 2-methylamino |
| | NSC 9406 |
| **Inchi:** | InChI=1S/C9H11NO2/c1-10-8-6-4-3-5-7(8)9(11)12-2/h3-6,10H,1-2H3 |
| **InchiKey:** | GVOWHGSUZUUUDR-UHFFFAOYSA-N |
| **Formula:** | C9H11NO2 |
| **SMILES:** | CNc1ccccc1C(=O)OC |
| **Mol. weight [g/mol]:** | 165.19 |
| **CAS:** | 85-91-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -16.85 | kJ/mol | Joback Method |
| hf | -195.36 | kJ/mol | Joback Method |
| hfus | 20.60 | kJ/mol | Joback Method |
| hvap | 54.16 | kJ/mol | Joback Method |
| log10ws | -1.72 | | Crippen Method |
| logp | 1.515 | | Crippen Method |
| mcvol | 131.330 | ml/mol | McGowan Method |
| pc | 3431.89 | kPa | Joback Method |

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|---|---|---|---|
| rinpol | 1407.90 | | NIST Webbook |
| rinpol | 1385.00 | | NIST Webbook |
| rinpol | 1385.00 | | NIST Webbook |
| rinpol | 1407.00 | | NIST Webbook |
| rinpol | 1408.00 | | NIST Webbook |
| rinpol | 1404.00 | | NIST Webbook |
| rinpol | 1412.00 | | NIST Webbook |
| rinpol | 1412.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1404.00 | | NIST Webbook |
| rinpol | 1388.00 | | NIST Webbook |
| rinpol | 1410.00 | | NIST Webbook |
| rinpol | 1406.00 | | NIST Webbook |
| rinpol | 1427.00 | | NIST Webbook |
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| rinpol | 1402.00 | | NIST Webbook |
| rinpol | 1375.00 | | NIST Webbook |
| rinpol | 1385.00 | | NIST Webbook |
| rinpol | 1385.00 | | NIST Webbook |
| rinpol | 1389.00 | | NIST Webbook |
| ripol | 2035.00 | | NIST Webbook |
| ripol | 2068.00 | | NIST Webbook |
| ripol | 2104.00 | | NIST Webbook |
| ripol | 2042.00 | | NIST Webbook |
| ripol | 2123.00 | | NIST Webbook |
| ripol | 2082.00 | | NIST Webbook |
| ripol | 2050.00 | | NIST Webbook |
| ripol | 2118.00 | | NIST Webbook |
| ripol | 2082.00 | | NIST Webbook |
| ripol | 2055.00 | | NIST Webbook |
| ripol | 2082.00 | | NIST Webbook |
| ripol | 2082.00 | | NIST Webbook |
| ripol | 2072.00 | | NIST Webbook |
| ripol | 2033.00 | | NIST Webbook |
| tb | 563.44 | K | Joback Method |
| tc | 780.85 | K | Joback Method |
| tf | 354.95 | K | Joback Method |
| vc | 0.490 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 301.19 | J/mol×K | 563.44 | Joback Method |
| cpg | 313.64 | J/mol×K | 599.68 | Joback Method |
| cpg | 325.37 | J/mol×K | 635.91 | Joback Method |
| cpg | 336.41 | J/mol×K | 672.15 | Joback Method |
| cpg | 346.75 | J/mol×K | 708.38 | Joback Method |
| cpg | 356.42 | J/mol×K | 744.62 | Joback Method |
| cpg | 365.43 | J/mol×K | 780.85 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C85916&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**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