# 3-METHOXYACETANILIDE

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|---|---|
| **Other names:** | 3'-Methoxyacetanilide |
| | Acetamide, N-(3-methoxyphenyl)- |
| | Acetanilide, 3'-methoxy- |
| | Aceto-m-anisidide |
| | N-(3-Methoxyphenyl)acetic acid amide |
| | N-Acetyl-m-anisidine |
| | m-Acetanisidide |
| | m-Acetanisidine |
| | m-Methoxyacetanilide |
| **Inchi:** | InChI=1S/C9H11NO2/c1-7(11)10-8-4-3-5-9(6-8)12-2/h3-6H,1-2H3,(H,10,11) |
| **InchiKey:** | OIEFZHJNURGFFI-UHFFFAOYSA-N |
| **Formula:** | C9H11NO2 |
| **SMILES:** | COc1cccc(NC(C)=O)c1 |
| **Mol. weight [g/mol]:** | 165.19 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -275.08 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 20.60 | kJ/mol | Joback Method |
| hvap | 75.05 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.92 | eV | Cheméo Relay (1.0) |
| log10ws | -1.92 | | Cheméo Relay (1.0) |
| logp | 1.654 | | Crippen Method |
| mcvol | 131.330 | ml/mol | McGowan Method |
| tb | 565.62 | K | Cheméo Relay (1.0) |
| tc | 788.27 | K | Cheméo Relay (1.0) |
| tf | 337.51 | K | Cheméo Relay (1.0) |

# 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 |

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|---|---|---|---|---|
| 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

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| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C588169&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |