# 4-Methoxy-3-methylphenylacetonitrile

**Inchi:** InChI=1S/C10H11NO/c1-8-7-9(5-6-11)3-4-10(8)12-2/h3-4,7H,5H2,1-2H3
**InchiKey:** QOMACJMHUFTRJI-UHFFFAOYSA-N
**Formula:** C10H11NO
**SMILES:** COc1ccc(CC#N)cc1C
**Mol. weight [g/mol]:** 161.20
**CAS:** 75391-57-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 154.65 | kJ/mol | Joback Method |
| hf | -3.48 | kJ/mol | Joback Method |
| hfus | 17.61 | kJ/mol | Joback Method |
| hvap | 54.34 | kJ/mol | Joback Method |
| log10ws | -2.74 | | Crippen Method |
| logp | 2.070 | | Crippen Method |
| mcvol | 135.250 | ml/mol | McGowan Method |
| pc | 2715.50 | kPa | Joback Method |
| tb | 589.34 | K | Joback Method |
| tc | 811.87 | K | Joback Method |
| tf | 341.14 | K | Joback Method |
| vc | 0.531 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 309.79 | J/mol×K | 589.34 | Joback Method |
| cpg | 321.57 | J/mol×K | 626.43 | Joback Method |
| cpg | 332.71 | J/mol×K | 663.52 | Joback Method |
| cpg | 343.21 | J/mol×K | 700.61 | Joback Method |
| cpg | 353.09 | J/mol×K | 737.69 | Joback Method |
| cpg | 362.34 | J/mol×K | 774.78 | Joback Method |
| cpg | 370.99 | J/mol×K | 811.87 | 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=C75391570&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |