# 3-Ethoxy-4-methoxyphenylacetonitrile

**Inchi:** InChI=1S/C11H13NO2/c1-3-14-11-8-9(6-7-12)4-5-10(11)13-2/h4-5,8H,3,6H2,1-2H3
**InchiKey:** DULUKHADKMYILX-UHFFFAOYSA-N
**Formula:** C11H13NO2
**SMILES:** CCOc1cc(CC#N)ccc1OC
**Mol. weight [g/mol]:** 191.23
**CAS:** 103796-99-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 58.07 | kJ/mol | Joback Method |
| hf | -156.34 | kJ/mol | Joback Method |
| hfus | 21.39 | kJ/mol | Joback Method |
| hvap | 58.98 | kJ/mol | Joback Method |
| log10ws | -2.80 | | Crippen Method |
| logp | 2.160 | | Crippen Method |
| mcvol | 155.210 | ml/mol | McGowan Method |
| pc | 2421.88 | kPa | Joback Method |
| tb | 634.64 | K | Joback Method |
| tc | 850.55 | K | Joback Method |
| tf | 374.64 | K | Joback Method |
| vc | 0.606 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 380.69 | J/mol×K | 634.64 | Joback Method |
| cpg | 393.20 | J/mol×K | 670.62 | Joback Method |
| cpg | 405.04 | J/mol×K | 706.61 | Joback Method |
| cpg | 416.20 | J/mol×K | 742.59 | Joback Method |
| cpg | 426.67 | J/mol×K | 778.58 | Joback Method |
| cpg | 436.45 | J/mol×K | 814.56 | Joback Method |
| cpg | 445.54 | J/mol×K | 850.55 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C103796992&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 |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |