# m-Nitrobenzylidene-2,5-dimethylphenylacetonitril

**Inchi:** InChI=1S/C17H14N2O2/c1-12-6-7-13(2)17(8-12)15(11-18)9-14-4-3-5-16(10-14)19(20)21
**InchiKey:** WAEYMLZYPBKJJR-DHDCSXOGSA-N
**Formula:** C17H14N2O2
**SMILES:** Cc1ccc(C)c(C(C#N)=Cc2cccc([N+](=O)[O-])c2)c1
**Mol. weight [g/mol]:** 278.31
**CAS:** 31881-16-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -8830.00 | kJ/mol | NIST Webbook |
| chs | -8826.44 | kJ/mol | NIST Webbook |
| gf | 528.59 | kJ/mol | Joback Method |
| hf | 305.99 | kJ/mol | Joback Method |
| hfs | 136.00 | kJ/mol | NIST Webbook |
| hfs | 136.50 | kJ/mol | NIST Webbook |
| hfus | 38.46 | kJ/mol | Joback Method |
| hvap | 87.08 | kJ/mol | Joback Method |
| log10ws | -5.96 | | Crippen Method |
| logp | 4.276 | | Crippen Method |
| mcvol | 217.370 | ml/mol | McGowan Method |
| pc | 2086.93 | kPa | Joback Method |
| tb | 914.62 | K | Joback Method |
| tc | 1182.06 | K | Joback Method |
| tf | 561.31 | K | Joback Method |
| vc | 0.861 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 620.33 | J/mol×K | 914.62 | Joback Method |
| cpg | 632.10 | J/mol×K | 959.19 | Joback Method |
| cpg | 642.94 | J/mol×K | 1003.77 | Joback Method |
| cpg | 652.98 | J/mol×K | 1048.34 | Joback Method |
| cpg | 662.34 | J/mol×K | 1092.91 | Joback Method |

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|---|---|---|---|---|
| cpg | 671.13 | J/mol×K | 1137.49 | Joback Method |
| cpg | 679.48 | J/mol×K | 1182.06 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C31881160&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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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |