# 2,4-Dimethylphenylacetonitrile

**Inchi:** InChI=1S/C10H11N/c1-8-3-4-10(5-6-11)9(2)7-8/h3-4,7H,5H2,1-2H3
**InchiKey:** OOWISQLTVOZJJI-UHFFFAOYSA-N
**Formula:** C10H11N
**SMILES:** Cc1ccc(CC#N)c(C)c1
**Mol. weight [g/mol]:** 145.20
**CAS:** 68429-53-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 259.65 | kJ/mol | Joback Method |
| hf | 128.74 | kJ/mol | Joback Method |
| hfus | 16.43 | kJ/mol | Joback Method |
| hvap | 51.93 | kJ/mol | Joback Method |
| log10ws | -3.09 | | Crippen Method |
| logp | 2.370 | | Crippen Method |
| mcvol | 129.380 | ml/mol | McGowan Method |
| pc | 2764.26 | kPa | Joback Method |
| tb | 566.92 | K | Joback Method |
| tc | 792.35 | K | Joback Method |
| tf | 318.91 | K | Joback Method |
| vc | 0.513 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 286.99 | J/mol×K | 566.92 | Joback Method |
| cpg | 298.92 | J/mol×K | 604.49 | Joback Method |
| cpg | 310.17 | J/mol×K | 642.06 | Joback Method |
| cpg | 320.73 | J/mol×K | 679.64 | Joback Method |
| cpg | 330.66 | J/mol×K | 717.21 | Joback Method |
| cpg | 339.96 | J/mol×K | 754.78 | Joback Method |
| cpg | 348.66 | J/mol×K | 792.35 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C68429538&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 |