# 2-Methylindoline

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|---|---|
| **Other names:** | 1H-Indole, 2,3-dihydro-2-methyl- |
| | «alpha»-Methyldihydroindole |
| | Dihydroindole, 2-methyl- |
| | Indoline, 2-methyl- |
| | 2-Methyl-2,3-dihydroindole |
| | 2,3-Dihydro-2-methylindole |
| | 2,3-Dihydro-2-methyl-1H-indole |
| | PE-11 |
| | NSC 65598 |
| **Inchi:** | InChI=1S/C9H11N/c1-7-6-8-4-2-3-5-9(8)10-7/h2-5,7,10H,6H2,1H3 |
| **InchiKey:** | QRWRJDVVXAXGBT-UHFFFAOYSA-N |
| **Formula:** | C9H11N |
| **SMILES:** | CC1Cc2ccccc2N1 |
| **Mol. weight [g/mol]:** | 133.19 |
| **CAS:** | 6872-06-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 276.14 | kJ/mol | Joback Method |
| hf | 106.58 | kJ/mol | Joback Method |
| hfus | 20.44 | kJ/mol | Joback Method |
| hvap | 45.24 | kJ/mol | Joback Method |
| log10ws | -2.29 | | Crippen Method |
| logp | 2.043 | | Crippen Method |
| mcvol | 113.030 | ml/mol | McGowan Method |
| pc | 3853.09 | kPa | Joback Method |
| tb | 492.27 | K | Joback Method |
| tc | 725.45 | K | Joback Method |
| tf | 353.10 | K | Joback Method |
| vc | 0.425 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 240.67 | J/mol×K | 492.27 | Joback Method |
| cpg | 255.54 | J/mol×K | 531.13 | Joback Method |
| cpg | 269.41 | J/mol×K | 570.00 | Joback Method |
| cpg | 282.35 | J/mol×K | 608.86 | Joback Method |
| cpg | 294.40 | J/mol×K | 647.72 | Joback Method |
| cpg | 305.62 | J/mol×K | 686.59 | Joback Method |
| cpg | 316.08 | J/mol×K | 725.45 | Joback Method |

# Sources

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|---|---|
| **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=C6872066&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |