# 3H-Indole, 2,3,3-trimethyl-

**Other names:** 2,3,3-Trimethyl-3H-indole
2,3,3-Trimethylindolenine
**Inchi:** InChI=1S/C11H13N/c1-8-11(2,3)9-6-4-5-7-10(9)12-8/h4-7H,1-3H3
**InchiKey:** FLHJIAFUWHPJRT-UHFFFAOYSA-N
**Formula:** C11H13N
**SMILES:** CC1=Nc2ccccc2C1(C)C
**Mol. weight [g/mol]:** 159.23
**CAS:** 1640-39-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 336.89 | kJ/mol | Joback Method |
| hf | 160.01 | kJ/mol | Joback Method |
| hfus | 15.71 | kJ/mol | Joback Method |
| hvap | 48.94 | kJ/mol | Joback Method |
| log10ws | -2.83 | | Crippen Method |
| logp | 3.070 | | Crippen Method |
| mcvol | 136.910 | ml/mol | McGowan Method |
| pc | 3224.64 | kPa | Joback Method |
| tb | 501.50 ± 0.50 | K | NIST Webbook |
| tc | 790.08 | K | Joback Method |
| tf | 379.33 | K | Joback Method |
| vc | 0.533 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 328.93 | J/mol×K | 547.56 | Joback Method |
| cpg | 345.19 | J/mol×K | 587.98 | Joback Method |
| cpg | 360.25 | J/mol×K | 628.40 | Joback Method |
| cpg | 374.29 | J/mol×K | 668.82 | Joback Method |
| cpg | 387.46 | J/mol×K | 709.24 | Joback Method |
| cpg | 399.96 | J/mol×K | 749.66 | Joback Method |
| cpg | 411.94 | J/mol×K | 790.08 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 501.70 | K | 99.20 | NIST Webbook |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1640397&Units=SI |

# 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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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