# Isoquinoline, 3-methyl-

**Other names:** 3-Methylisoquinoline
**Inchi:** InChI=1S/C10H9N/c1-8-6-9-4-2-3-5-10(9)7-11-8/h2-7H,1H3
**InchiKey:** FVVXWRGARUACNW-UHFFFAOYSA-N
**Formula:** C10H9N
**SMILES:** Cc1cc2ccccc2cn1
**Mol. weight [g/mol]:** 143.19
**CAS:** 1125-80-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3510 | | KDB |
| ie | 8.11 | eV | NIST Webbook |
| ie | 7.74 ± 0.02 | eV | NIST Webbook |
| log10ws | -3.52 | | Crippen Method |
| logp | 2.543 | | Crippen Method |
| mcvol | 118.520 | ml/mol | McGowan Method |
| pc | 5100.00 | kPa | KDB |
| rinpol | 1322.00 | | NIST Webbook |
| rinpol | 1313.00 | | NIST Webbook |
| tb | 519.20 | K | NIST Webbook |
| tb | 526.40 | K | KDB |
| tb | 526.28 ± 0.07 | K | NIST Webbook |
| tb | 526.30 ± 0.23 | K | NIST Webbook |
| tb | 519.15 ± 0.60 | K | NIST Webbook |
| tc | 808.00 | K | KDB |
| tf | 336.80 ± 0.30 | K | NIST Webbook |
| tf | 336.50 ± 0.20 | K | NIST Webbook |
| tf | 337.00 | K | KDB |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |

| | |
|---|---|
| Coeff. A | 1.41766e+01 |
| Coeff. B | -4.13771e+03 |
| Coeff. C | -8.63080e+01 |
| Temperature range (K), min. | 384.22 |
| Temperature range (K), max. | 553.05 |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1366 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125800&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |