# 2H-Benzotriazole, 2-methyl-

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|---|---|
| **Other names:** | 2-Methylbenzotriazole |
| | 2-Methyl-2H-benzotriazole |
| **Inchi:** | InChI=1S/C7H7N3/c1-10-8-6-4-2-3-5-7(6)9-10/h2-5H,1H3 |
| **InchiKey:** | PWORFEDVDWBHSJ-UHFFFAOYSA-N |
| **Formula:** | C7H7N3 |
| **SMILES:** | Cn1nc2ccccc2n1 |
| **Mol. weight [g/mol]:** | 133.15 |
| **CAS:** | 16584-00-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 890.10 | kJ/mol | NIST Webbook |
| basg | 855.90 | kJ/mol | NIST Webbook |
| ie | 8.54 | eV | NIST Webbook |
| log10ws | -4.10 | | Crippen Method |
| logp | 0.968 | | Crippen Method |
| mcvol | 100.510 | ml/mol | McGowan 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=C16584002&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume