# Gramine

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|---|---|
| **Other names:** | 1H-Indole-3-methanamine, N,N-dimethyl-<br>Indole, 3-[(dimethylamino)methyl]-<br>Donaxin<br>Donaxine<br>Gramin<br>3-[(Dimethylamino)methyl]indole<br>«beta»-Dimethylaminomethylindole<br>beta-(Dimethylaminomethyl)indole<br>3-(N,N-Dimethylaminomethyl)indole<br>N,N-Dimethyl-1H-indole-3-methylamine<br>(1H-Indol-3-ylmethyl)-dimethyl-amine<br>NSC 16892<br>b-(Dimethylaminomethyl)indole<br>3-Dimethylaminomethylindol (gramin)<br>1H-Indol-3-yl-N,N-dimethylmethanamine<br>indol-3-ylmethyldimethylamine |
| **Inchi:** | InChI=1S/C11H14N2/c1-13(2)8-9-7-12-11-6-4-3-5-10(9)11/h3-7,12H,8H2,1-2H3 |
| **InchiKey:** | OCDGBSUVYYVKQZ-UHFFFAOYSA-N |
| **Formula:** | C11H14N2 |
| **SMILES:** | CN(C)Cc1c[nH]c2ccccc12 |
| **Mol. weight [g/mol]:** | 174.24 |
| **CAS:** | 87-52-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 7.69 ± 0.16 | eV | NIST Webbook |
| log10ws | -2.78 | | Crippen Method |
| logp | 1.748 | | Crippen Method |
| mcvol | 146.890 | ml/mol | McGowan Method |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1622.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C87525&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |