

1H-Indole-3-ethanamine, «alpha»-methyl-

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|-----------------------------|---|
| Other names: | 3-(2-Aminopropyl)indole 164 E Indole, 3-(2-aminopropyl)- «alpha»-Methyl-3-indoleethanamine «alpha»-Methyltryptamine Ro 3-0926 U 14 «alpha»-Methyl-«beta»-indoleethylamine U-14164E(dl) Indopan IT-290(dl) IT-403(D) U 14164 E AMT Tryptamine, «alpha»-methyl NSC 97069 DL-3-(2-aminopropyl)indole |
| Inchi: | InChI=1S/C11H14N2/c1-8(12)6-9-7-13-11-5-3-2-4-10(9)11/h2-5,7-8,13H,6,12H2,1H3 |
| InchiKey: | QSQQQURBVYWZKJ-UHFFFAOYSA-N |
| Formula: | C11H14N2 |
| SMILES: | CC(N)Cc1c[nH]c2ccccc12 |
| Mol. weight [g/mol]: | 174.24 |
| CAS: | 299-26-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.26 | | Crippen Method |
| logp | 1.576 | | Crippen Method |
| mcvol | 146.890 | ml/mol | McGowan Method |
| rinpol | 1740.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C299263&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpolar: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/50-677-5/1H-Indole-3-ethanamine-alpha-methyl.pdf>

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