

1H-Indazole, 3-methoxy-

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|-----------------------------|--|
| Other names: | 3-Methoxyindazole |
| Inchi: | InChI=1S/C8H8N2O/c1-11-8-6-4-2-3-5-7(6)9-10-8/h2-5H,1H3,(H,9,10) |
| InchiKey: | DHIHZLGSYHTLMS-UHFFFAOYSA-N |
| Formula: | C8H8N2O |
| SMILES: | COc1n[nH]c2cccc12 |
| Mol. weight [g/mol]: | 148.16 |
| CAS: | 1848-41-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.38 | | Crippen Method |
| logp | 1.090 | | Crippen Method |
| mcvol | 110.490 | ml/mol | McGowan Method |
| rinpol | 1699.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C1848415&Units=SI |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-763-7/1H-Indazole-3-methoxy.pdf>

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