

2,3-Diphenylindole

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|-----------------------------|---|
| Other names: | 1H-Indole, 2,3-diphenyl- Indole, 2,3-diphenyl- 2,3-diphenyl-1H-indole |
| Inchi: | InChI=1S/C20H15N/c1-3-9-15(10-4-1)19-17-13-7-8-14-18(17)21-20(19)16-11-5-2-6-12-1 |
| InchiKey: | GYGKJNGSQORRG-UHFFFAOYSA-N |
| Formula: | C20H15N |
| SMILES: | <chem>c1ccc(-c2[nH]c3ccccc3c2-c2ccccc2)cc1</chem> |
| Mol. weight [g/mol]: | 269.34 |
| CAS: | 3469-20-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.70 | | Crippen Method |
| logp | 5.020 | | Crippen Method |
| mcvol | 216.200 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=C3469203&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/66-804-6/2-3-Diphenylindole.pdf>

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