

N-(Diphenylcarbamoyl)piperidine

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|-----------------------------|--|
| Inchi: | InChI=1S/C18H20N2O/c21-18(19-14-8-3-9-15-19)20(16-10-4-1-5-11-16)17-12-6-2-7-13- |
| InchiKey: | DKMZFFROTTLIPQ-UHFFFAOYSA-N |
| Formula: | C18H20N2O |
| SMILES: | O=C(N1CCCCC1)N(c1ccccc1)c1ccccc1 |
| Mol. weight [g/mol]: | 280.36 |
| CAS: | 75534-73-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.49 | | Crippen Method |
| logp | 4.431 | | Crippen Method |
| mcvol | 227.630 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C75534735&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 |

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<https://www.chemeo.com/cid/99-477-4/N-Diphenylcarbamoyl-piperidine.pdf>

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