

1-(Diphenyl methyl)-pyridinium

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|-----------------------------|---|
| Inchi: | InChI=1S/C18H16N/c1-4-10-16(11-5-1)18(17-12-6-2-7-13-17)19-14-8-3-9-15-19/h1-15,1 |
| InchiKey: | NOIXUZSKNIAJKZ-UHFFFAOYSA-N |
| Formula: | C18H16N |
| SMILES: | c1ccc(C(c2ccccc2)[n+]2ccccc2)cc1 |
| Mol. weight [g/mol]: | 246.33 |
| CAS: | 46957-56-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.15 | | Crippen Method |
| logp | 3.612 | | Crippen Method |
| mcvol | 205.330 | 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=C46957566&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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/70-477-5/1-Diphenyl-methyl-pyridinium.pdf>

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