

Hexahydro-3,3,5-trimethyl-2-p-tolyl-1,4,2-diazaphosphorinane

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|-----------------------------|--|
| Inchi: | InChI=1S/C13H21N2OP/c1-10-5-7-12(8-6-10)17(16)13(3,4)15-11(2)9-14-17/h5-8,11,15H |
| InchiKey: | FARMSTZLWUOGFG-UHFFFAOYSA-N |
| Formula: | C13H21N2OP |
| SMILES: | Cc1ccc(P2(=O)NCC(C)NC2(C)C)cc1 |
| Mol. weight [g/mol]: | 252.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.09 | | Crippen Method |
| logp | 2.216 | | Crippen Method |
| mcvol | 205.700 | ml/mol | McGowan Method |
| rinpol | 2178.00 | | NIST Webbook |
| rinpol | 2178.00 | | 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=R566873&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 |

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