

N,n'-bis-(4-(6-methyl)1,3,3a,7-tetrazaindenyl)-4,4'-biphenyl

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C24H20N10/c1-15-11-21(33-23(29-15)25-13-27-33)31-19-7-3-17(4-8-19)18-5- |
| InchiKey: | QJXJILSHCXYOAB-UHFFFAOYSA-N |
| Formula: | C24H20N10 |
| SMILES: | Cc1cc(Nc2ccc(-c3ccc(Nc4cc(C)nc5ncnn45)cc3)cc2)n2ncnc2n1 |
| Mol. weight [g/mol]: | 448.48 |
| CAS: | 116008-06-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.15 | | Crippen Method |
| logp | 4.333 | | Crippen Method |
| mcvol | 323.460 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116008061&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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

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