

Pyridine, 4-((1-pyrenylimino)-methyl)-

Inchi: InChI=1S/C22H14N2/c1-2-16-4-5-18-7-9-20(24-14-15-10-12-23-13-11-15)19-8-6-17(3-1)
InchiKey: RPQVYYCWTCHISJ-ZVHZXABRSA-N
Formula: C22H14N2
SMILES: C(=Nc1ccc2ccc3cccc4ccc1c2c34)c1ccncc1
Mol. weight [g/mol]: 306.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.93 | | Crippen Method |
| logp | 5.730 | | Crippen Method |
| mcvol | 234.900 | ml/mol | McGowan Method |

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=B6008109&Units=SI>

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/53-300-9/Pyridine-4-1-pyrenylimino-methyl.pdf>

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