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/ci990307l
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