

# 2,3,10,11-Tetrahydrobenzo[b]dipyrido[3,2,1-de:1,2

<b>Inchi:</b>	InChI=1S/C22H16N2O2/c25-17-9-11-23-15-7-3-4-8-16(15)24-12-10-18(26)20-14-6-2-1-5
<b>InchiKey:</b>	CJVPWNJSVOPLPU-UHFFFAOYSA-N
<b>Formula:</b>	C22H16N2O2
<b>SMILES:</b>	O=C1CCN2c3ccccc3N3CCC(=O)c4c3c2c1c1cccc41
<b>Mol. weight [g/mol]:</b>	340.37
<b>CAS:</b>	100436-05-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	4.602		Crippen Method
mcvol	244.380	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C100436053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C100436053&amp;Units=SI</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/51-500-9/2-3-10-11-Tetrahydrobenzo-b-dipyrido-3-2-1-de-1-2-3-mn-phenazine-1-12-dic>

Generated by Cheméo on 2024-04-29 19:13:28.949279277 +0000 UTC m=+16707257.869856590.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.