

# 2,4-Diacetoxy-10-cyanoazuleno(2,1-b)pyridine

<b>Inchi:</b>	InChI=1S/C18H12N2O4/c1-10(21)23-15-8-16(24-11(2)22)20-18-14(9-19)12-6-4-3-5-7-13
<b>InchiKey:</b>	LZZFYPTNVKRBH-UHFFFAOYSA-N
<b>Formula:</b>	C18H12N2O4
<b>SMILES:</b>	CC(=O)Oc1cc(OC(C)=O)c2c3ccccc-3c(C#N)c2n1
<b>Mol. weight [g/mol]:</b>	320.30
<b>CAS:</b>	53299-93-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	3.062		Crippen Method
mcvol	228.040	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53299937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53299937&amp;Units=SI</a>
<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>

## 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

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