

2,4-DIACETOXY-10-CYANOAZULENO(2,1-B)PYRIDINE

Inchi:	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
InchiKey:	LZZFYPFTNVKRBH-UHFFFAOYSA-N
Formula:	C18H12N2O4
SMILES:	CC(=O)Oc1cc(OC(C)=O)c2c3cccccc-3c(C#N)c2n1
Mol. weight [g/mol]:	320.30

Physical Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53299937&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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