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

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