

1-Acetyl-2,3-phthaloylpyrrocoline

Inchi:	InChI=1S/C18H11NO3/c1-10(20)14-13-8-4-5-9-19(13)16-15(14)17(21)11-6-2-3-7-12(11)
InchiKey:	OLBAGJDDSBANJY-UHFFFAOYSA-N
Formula:	C18H11NO3
SMILES:	CC(=O)c1c2c(n3ccccc13)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	289.28
CAS:	98596-11-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	2.917		Crippen Method
mcvol	205.630	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=C98596113&Units=SI

Legend

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

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<https://www.chemeo.com/cid/97-362-3/1-Acetyl-2-3-phthaloylpyrrocoline.pdf>

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