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