1-Carbomethoxy-2,3-phthaloylpyrrocoline

Inchi: InChI=1S/C18H11NO4/c1-23-18(22)13-12-8-4-5-9-19(12)15-14(13)16(20)10-6-2-3-7-11(
InchiKey: HJDHYWBGLVTHKF-UHFFFAOYSA-N
Formula: C18H11NO4
SMILES: COC(=O)c1c2c(n3ccccc13)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 305.28
CAS: 98596-13-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	2.501		Crippen Method
mcvol	211.500	ml/mol	McGowan Method

Sources

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=C98596135&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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