1-Carboethoxy-2,3-phthaloylpyrrocoline

Inchi:	InChI=1S/C19H13NO4/c1-2-24-19(23)14-13-9-5-6-10-20(13)16-15(14)17(21)11-7-3-4-8-
InchiKey:	RCDIUAFMNCXJRV-UHFFFAOYSA-N
Formula:	C19H13NO4
SMILES:	CCOC(=O)c1c2c(n3ccccc13)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	319.31
CAS:	3306-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	2.891		Crippen Method
mcvol	225.590	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3306932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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