1-Phenylcarbamoyl-2,3-phthaloylpyrrocoline

Other names: 6,11-dihydro-6,11-dioxo-N-phenylbenzo[f]pyrido[1,2-a]indole-12-carboxamide
Inchi: InChI=1S/C23H14N2O3/c26-21-15-10-4-5-11-16(15)22(27)20-19(21)18(17-12-6-7-13-25
InchiKey: UQCAZSLFSDIWBA-UHFFFAOYSA-N
Formula: C23H14N2O3
SMILES: O=C1c2ccccc2C(=O)c2c1c(C(=O)Nc1ccccc1)c1ccccn21
Mol. weight [g/mol]: 366.37
CAS: 3135-54-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.57		Crippen Method
logp	3.967		Crippen Method
mcvol	262.300	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=C3135544&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

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