

1-Phenylcarbamoyl-2,3-phthaloyl-7,8-benzopyrrocoline

Inchi:	InChI=1S/C27H16N2O3/c30-25-19-12-6-7-13-20(19)26(31)24-21(25)22(27(32)28-17-9-2
InchiKey:	RCEMTSCJFPZWPN-UHFFFAOYSA-N
Formula:	C27H16N2O3
SMILES:	O=C1c2ccccc2C(=O)c2c1c(C(=O)Nc1cccc1)c1c3ccccc3ccn21
Mol. weight [g/mol]:	416.43
CAS:	15208-30-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	5.120		Crippen Method
mcvol	299.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C15208307&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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