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

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)Nc1ccccc1)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/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=C15208307&Units=SI

Legend

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