

1-Phenylcarbamoyl-7-styryl-2,3-phthaloylpyrrocol

Inchi:	InChI=1S/C31H20N2O3/c34-29-23-13-7-8-14-24(23)30(35)28-27(29)26(31(36)32-22-11-
InchiKey:	TVXUATWJBWGMZOZ-UHFFFAOYSA-N
Formula:	C31H20N2O3
SMILES:	O=C1c2ccccc2C(=O)c2c1c(C(=O)Nc1cccc1)c1cc(C=Cc3ccccc3)ccn21
Mol. weight [g/mol]:	468.50
CAS:	104601-60-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.17		Crippen Method
logp	6.137		Crippen Method
mcvol	346.960	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=C104601607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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<https://www.chemeo.com/cid/29-114-3/1-Phenylcarbamoyl-7-styryl-2-3-phthaloylpyrrocoline.pdf>

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