# 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:** TVXUATWJBWGMOZ-UHFFFAOYSA-N
**Formula:** C31H20N2O3
**SMILES:** O=C1c2ccccc2C(=O)c2c1c(C(=O)Nc1ccccc1)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/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