Pyrrolidine, 1-(2,3-dihydro-4-pheynl-1(4h)-benzopyran-4-carbo

Inchi: InChI=1S/C20H21NO2/c22-19(21-13-6-7-14-21)20(16-8-2-1-3-9-16)12-15-23-18-11-5-4-

InchiKey: BXDFGVWVCDGMAT-UHFFFAOYSA-N

Formula: C20H21NO2

SMILES: O=C(N1CCCC1)C1(c2ccccc2)CCOc2ccccc21

Mol. weight [g/mol]: 307.39

CAS: 94684-96-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	3.378		Crippen Method
mcvol	240.840	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=C94684965&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