

# Pyrrolidine, 1-(2,3-dihydro-4-phenyl-1(4h)-benzopyran-4-carbonyl)

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:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C94684965&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94684965&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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