Pyrrolidine, 1-[4-(4-chlorophenyl)-3-phenyl-2-butenyl]-

Other names: Pyrrobutamide
Pyrrolidine, 1-[«gamma»-(p-chlorobenzyl)cinnamyl]-
Copyronil
Pyrrobutamine
1-(4-(4-chlorophenyl)-3-phenylbut-2-enyl)pyrrolidine

Inchi: InChI=1S/C20H22ClN/c21-20-10-8-17(9-11-20)16-19(18-6-2-1-3-7-18)12-15-22-13-4-5-1

InchiKey: WDYYVNNRTDZKAZ-UNOMPAQXSA-N

Formula: C20H22ClN

SMILES: Clc1ccc(CC(=CCN2CCCC2)c2ccccc2)cc1

Mol. weight [g/mol]: 311.85

CAS: 91-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	5.062		Crippen Method
mcvol	252.200	ml/mol	McGowan Method
rinpol	2419.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2428.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2428.00		NIST Webbook
rinpol	2430.00		NIST Webbook
ripol	3270.00		NIST Webbook
ripol	3270.00		NIST Webbook

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=C91827&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices