Quinoline, 2-[2-(4-chlorophenyl)ethenyl]-

Other names:	Quinoline, 2-(p-chlorostyryl)-
	2-[2-(4-Chlorophenyl)ethenyl]quinoline
	2-p-Chlorostyryl quinoline
Inchi:	InChI=1S/C17H12ClN/c18-15-9-5-13(6-10-15)7-11-16-12-8-14-3-1-2-4-17(14)19-16/h1-1
InchiKey:	PWZHLFSCFYMSMR-YRNVUSSQSA-N
Formula:	C17H12ClN
SMILES:	Clc1ccc(C=Cc2ccc3ccccc3n2)cc1
Mol. weight [g/mol]:	265.74
CAS:	5392-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	5.059		Crippen Method
mcvol	201.330	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=C5392198&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

Latest version available from:
https://www.chemeo.com/cid/82-864-2/Quinoline-2-2-4-chlorophenyl-ethenyl.pdf

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