TICLOPIDINE

Other names:	Thieno(3,2-c)pyridine, 4,5,6,7-tetrahydro-5-((2-chlorophenyl)methyl)-
	5-((2-Chlorophenyl)methyl)-4,5,6,7-tetrahydrothieno(3,2-c)pyridine
	PCR 5332
	Ticlopidine
	5-(O-Chlorobenzyl)-4,5,6,7-tetrahydrothieno-[3,2-c]pyridine
Inchi:	InChI=1S/C14H14ClNS/c15-13-4-2-1-3-11(13)9-16-7-5-14-12(10-16)6-8-17-14/h1-4,6,8H
InchiKey:	PHWBOXQYWZNQIN-UHFFFAOYSA-N
Formula:	C14H14ClNS
SMILES:	Clc1ccccc1CN1CCc2sccc2C1
Mol. weight [g/mol]:	263.79

Physical Properties

Property code	Value	Unit	Source
logp	3.960		Crippen Method
mcvol	192.610	ml/mol	McGowan Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55142853&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices