

# Thieno[3,2-c]pyridine, 5-[(2-chlorophenyl)methyl]-4,5,6,7-tetrahydro-

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:** PHWBOXQYWZLNQIN-UHFFFAOYSA-N

**Formula:** C14H14ClNS

**SMILES:** Clc1ccccc1CN1CCc2sccc2C1

**Mol. weight [g/mol]:** 263.79

**CAS:** 55142-85-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.960		Crippen Method
mcvol	192.610	ml/mol	McGowan Method
rinsol	2090.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C55142853&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

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