2-(para-Chlorobenzyl)-pyridine

Other names:	2-(4-Chlorobenzyl)pyridine
	2-(p-Chlorobenzyl)pyridine
	Pyridine, 2-[(4-chlorophenyl)methyl]-
	2-[(4-Chlorophenyl)methyl]pyridine
	2-(4'-chlorobenzyl)pyridine
Inchi:	InChI=1S/C12H10ClN/c13-11-6-4-10(5-7-11)9-12-3-1-2-8-14-12/h1-8H,9H2
InchiKey:	XSVWMIMFDMJQRL-UHFFFAOYSA-N
Formula:	C12H10ClN
SMILES:	Clc1ccc(Cc2ccccn2)cc1
Mol. weight [g/mol]:	203.67
CAS:	4350-41-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.326		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.20	K	2.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4350418&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure