4-(P-CHLOROBENZYL)PYRIDINE

Other names:	4-(4-Chlorobenzyl)pyridine
	4-(p-Chlorobenzyl)pyridine
	Pyridine, 4-[(4-chlorophenyl)methyl]-
	4-(4'-chlorobenzyl)pyridine
Inchi:	InChI=1S/C12H10ClN/c13-12-3-1-10(2-4-12)9-11-5-7-14-8-6-11/h1-8H,9H2
InchiKey:	OHKBVLWPESSWKC-UHFFFAOYSA-N
Formula:	C12H10ClN
SMILES:	Clc1ccc(Cc2ccncc2)cc1
Mol. weight [g/mol]:	203.67

Physical Properties

Property code	Value	Unit	Source
af	0.4480		Cheméo Relay (1.0)
hf	187.00	kJ/mol	Cheméo Relay (1.0)
hvap	79.22	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
log10ws	-2.70		Cheméo Relay (1.0)
logp	3.326		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
pc	3411.74	kPa	Cheméo Relay (1.0, beta)
tb	593.52	K	Cheméo Relay (1.0)
tc	836.44	K	Cheméo Relay (1.0)
tf	323.75	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4409114&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point