Methanone,(2-chlorophenyl)-2-pyridinyl-

Other names: 2-(2-Chlorobenzoyl)-pyridine
Inchi: InChI=1S/C12H8ClNO/c13-10-6-2-1-5-9(10)12(15)11-7-3-4-8-14-11/h1-8H
InchiKey: XSPNJXJVXUZKPE-UHFFFAOYSA-N
Formula: C12H8ClNO
SMILES: O=C(c1ccccn1)c1ccccc1Cl
Mol. weight [g/mol]: 217.65
CAS: 1694-57-1

Physical Properties

Property code	Value	Unit	Source
ie	8.98	eV	NIST Webbook
log10ws	-3.88		Crippen Method
logp	2.966		Crippen Method
mcvol	156.210	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694571&Units=SI
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

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume