Methanone,(2-methylphenyl)-2-pyridinyl-

Other names:	2-(2-Methylbenzoyl)-pyridine
Inchi:	InChI=1S/C13H11NO/c1-10-6-2-3-7-11(10)13(15)12-8-4-5-9-14-12/h2-9H,1H3
InchiKey:	GWXTVPWMINBKEI-UHFFFAOYSA-N
Formula:	C13H11NO
SMILES:	Cc1ccccc1C(=O)c1ccccn1
Mol. weight [g/mol]:	197.23
CAS:	54523-78-3

Physical Properties

Property code	Value	Unit	Source
ie	8.72	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
log10ws	-3.67		Crippen Method
logp	2.621		Crippen Method
mcvol	158.060	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54523783&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

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