

Methanone, (2-fluorophenyl)-2-pyridinyl-

Other names:	Ketone, o-fluorophenyl 2-pyridyl 2-(2-Fluorobenzoyl)-pyridine
Inchi:	InChI=1S/C12H8FNO/c13-10-6-2-1-5-9(10)12(15)11-7-3-4-8-14-11/h1-8H
InchiKey:	NXJUUEIQHLXBPZ-UHFFFAOYSA-N
Formula:	C12H8FNO
SMILES:	O=C(c1cccn1)c1cccc1F
Mol. weight [g/mol]:	201.20
CAS:	6238-65-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.452		Crippen Method
mvol	145.740	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6238659&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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