

Ketone, methyl 6-methyl-2-pyridyl

Other names:	2-Acetyl-6-methylpyridine
Inchi:	InChI=1S/C8H9NO/c1-6-4-3-5-8(9-6)7(2)10/h3-5H,1-2H3
InchiKey:	FPQMUQPPAYCAME-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=O)c1cccc(C)n1
Mol. weight [g/mol]:	135.16
CAS:	6940-57-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.593		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
rinpol	1073.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1614.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6940574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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