

2-(2-Methylpropyl)-3,5-di(1-methylethyl)pyridine

Other names:	2-isobutyl-3,5-isopropyl-pyridine
Inchi:	InChI=1S/C15H25N/c1-10(2)7-15-14(12(5)6)8-13(9-16-15)11(3)4/h8-12H,7H2,1-6H3
InchiKey:	CZESXOCCJVKONH-UHFFFAOYSA-N
Formula:	C15H25N
SMILES:	CC(C)Cc1ncc(C(C)C)cc1C(C)C
Mol. weight [g/mol]:	219.37
CAS:	7033-68-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	4.527		Crippen Method
mcvol	208.430	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7033683&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
mcvol:	McGowan's characteristic volume

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