

Pyridine, 5-hexyl-2-methyl-

Inchi:	InChI=1S/C12H19N/c1-3-4-5-6-7-12-9-8-11(2)13-10-12/h8-10H,3-7H2,1-2H3
InchiKey:	CVQOAKGVDNOWHA-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CCCCCc1ccc(C)nc1
Mol. weight [g/mol]:	177.29
CAS:	710-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	3.513		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
rinpol	1410.00		NIST Webbook
ripol	1837.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C710407&Units=SI

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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<https://www.chemeo.com/cid/31-936-8/Pyridine-5-hexyl-2-methyl.pdf>

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