

Pyridine, 3-(1-buten-1-yl)-4-propyl, (E)-

Inchi:	InChI=1S/C12H17N/c1-3-5-7-12-10-13-9-8-11(12)6-4-2/h5,7-10H,3-4,6H2,1-2H3/b7-5+
InchiKey:	MUYDOEGEMIQLND-FNORWQNLSA-N
Formula:	C12H17N
SMILES:	CCC=Cc1cnccc1CCC
Mol. weight [g/mol]:	175.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.457		Crippen Method
mcvol	161.860	ml/mol	McGowan Method
rinpol	1438.00		NIST Webbook
rinpol	1442.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R68679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

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