Pyridine, 2-isopentyl-5-methyl

Inchi: InChI=1S/C11H17N/c1-9(2)4-6-11-7-5-10(3)8-12-11/h5,7-9H,4,6H2,1-3H3
InchiKey: JSPQTJXSMXIDKA-UHFFFAOYSA-N
Formula: C11H17N
SMILES: Cc1ccc(CCC(C)C)nc1
Mol. weight [g/mol]: 163.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.979		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
rinpol	1267.00		NIST Webbook
rinpol	1267.00		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=R555803&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.