6-methyl-2-pentylpyridine

Other names: Pyridine, 2-pentyl-6-methyl
Inchi: InChI=1S/C11H17N/c1-3-4-5-8-11-9-6-7-10(2)12-11/h6-7,9H,3-5,8H2,1-2H3
InchiKey: RTIQJSTXWLILMG-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCCCCc1cccc(C)n1
Mol. weight [g/mol]: 163.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	3.123		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
rinpol	1249.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1249.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U365952&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
rinpol: Non-polar retention indices