

4-(1-Ethylbutyl)pyridine

Inchi: InChI=1S/C11H17N/c1-3-5-10(4-2)11-6-8-12-9-7-11/h6-10H,3-5H2,1-2H3
InchiKey: MKNJSWGAZNYIAK-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCCC(CC)c1ccncc1
Mol. weight [g/mol]: 163.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	3.375		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook

Sources

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=R555794&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/57-370-8/4-1-Ethylbutyl-pyridine.pdf>

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