

Pyridine, 4-(1-methylbutyl)

Inchi: InChI=1S/C10H15N/c1-3-4-9(2)10-5-7-11-8-6-10/h5-9H,3-4H2,1-2H3
InchiKey: ZVXQINUALXERIW-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CCCC(C)c1ccncc1
Mol. weight [g/mol]: 149.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.985		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
rinpol	1167.00		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=R555858&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/40-429-1/Pyridine-4-1-methylbutyl.pdf>

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