

Pyridine, 4-(1-methylpropyl)

Inchi: InChI=1S/C9H13N/c1-3-8(2)9-4-6-10-7-5-9/h4-8H,3H2,1-2H3
InchiKey: HGMLMFWWXQNLLV-UHFFFAOYSA-N
Formula: C9H13N
SMILES: CCC(C)c1ccncc1
Mol. weight [g/mol]: 135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.595		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1128.00		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=R555863&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

Latest version available from:

<https://www.chemeo.com/cid/38-177-4/Pyridine-4-1-methylpropyl.pdf>

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