

Pyridine, 4-methyl-2-(1-methylethyl)

Inchi: InChI=1S/C9H13N/c1-7(2)9-6-8(3)4-5-10-9/h4-7H,1-3H3
InchiKey: IQTHCDAGRCAFJT-UHFFFAOYSA-N
Formula: C9H13N
SMILES: Cc1ccnc(C(C)C)c1
Mol. weight [g/mol]: 135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.513		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpola	1033.00		NIST Webbook
rinpola	1035.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68736&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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