

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

Inchi: InChI=1S/C9H11N/c1-7(2)9-4-5-10-8(3)6-9/h4-6H,1H2,2-3H3
InchiKey: CXGHVELUDDLRAP-UHFFFAOYSA-N
Formula: C9H11N
SMILES: C=C(C)c1ccnc(C)c1
Mol. weight [g/mol]: 133.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.423		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
rinpol	1097.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1097.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R68651&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

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<https://www.chemeo.com/cid/13-571-3/Pyridine-2-methyl-4-1-methylethenyl.pdf>

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