4-isopropenylpyridine

Other names: Pyridine, 4-(1-methylethenyl)
Inchi: InChI=1S/C8H9N/c1-7(2)8-3-5-9-6-4-8/h3-6H,1H2,2H3
InchiKey: MPMPYHKTFSOUHU-UHFFFAOYSA-N
Formula: C8H9N
SMILES: C=C(C)c1ccncc1
Mol. weight [g/mol]: 119.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	2.115		Crippen Method
mcvol	105.500	ml/mol	McGowan Method
rinpol	1031.00		NIST Webbook
rinpol	1034.00		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=R68718&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