Pyridine, 3-(1-butenyl), E

Other names: Pyridine, 3-(1-buten-1-yl), (E)-
Inchi: InChI=1S/C9H11N/c1-2-3-5-9-6-4-7-10-8-9/h3-8H,2H2,1H3/b5-3+
InchiKey: KTXMSWAHSUYOHZ-HWKANZROSA-N
Formula: C9H11N
SMILES: CCC=Cc1cccnc1
Mol. weight [g/mol]: 133.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.505		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
rinpol	1176.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	1657.00		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=R68697&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
ripol: Polar retention indices