

Pyridine, 3-ethenyl-

Other names:	Pyridine, 3-vinyl- 3-Vinylpyridine 3-Ethenylpyridine
Inchi:	InChI=1S/C7H7N/c1-2-7-4-3-5-8-6-7/h2-6H,1H2
InchiKey:	DPZYLEIWHTWHCU-UHFFFAOYSA-N
Formula:	C7H7N
SMILES:	C=Cc1ccnc1
Mol. weight [g/mol]:	105.14
CAS:	1121-55-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	1.725		Crippen Method
mcvol	91.410	ml/mol	McGowan Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	971.50		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=C1121557&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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