

Pyridine, 2-ethyl-5-methyl-

Other names:	2-Ethyl-5-methylpyridine 5-Methyl-2-ethyl pyridine
Inchi:	InChI=1S/C8H11N/c1-3-8-5-4-7(2)6-9-8/h4-6H,3H2,1-2H3
InchiKey:	COHDGTRFTKHYSJ-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccc(C)cn1
Mol. weight [g/mol]:	121.18
CAS:	18113-81-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.952		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1033.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1385.00		NIST Webbook
tb	447.15 ± 2.00	K	NIST Webbook

Sources

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=C18113810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/13-291-4/Pyridine-2-ethyl-5-methyl.pdf>

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