

Pyridine, 3-ethyl-2,5-dimethyl

Other names:	3-ethyl-2,5-dimethylpyridine
Inchi:	InChI=1S/C9H13N/c1-4-9-5-7(2)6-10-8(9)3/h5-6H,4H2,1-3H3
InchiKey:	PPSBKGGGGXWSAB-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCc1cc(C)cnc1C
Mol. weight [g/mol]:	135.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.261		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1084.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1124.00		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=R53561&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

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