

2-methyl-4,5-diethylpyridine

Inchi:	InChI=1S/C10H15N/c1-4-9-6-8(3)11-7-10(9)5-2/h6-7H,4-5H2,1-3H3
InchiKey:	CQOVHGCXVHWHBM-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCc1cnc(C)cc1CC
Mol. weight [g/mol]:	149.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	2.515		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
rinpol	1248.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142328&Units=SI
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

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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