

2,3-diethenyl-5-methylpyrazine

Inchi:	InChI=1S/C9H10N2/c1-4-8-9(5-2)11-7(3)6-10-8/h4-6H,1-2H2,3H3
InchiKey:	VQQLAWXMUPSVGA-UHFFFAOYSA-N
Formula:	C9H10N2
SMILES:	C=Cc1ncc(C)nc1C=C
Mol. weight [g/mol]:	146.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	2.071		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
rinpol	1172.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225884&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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