

2,5-dimethyl-3-propenylpyrazine

Inchi:	InChI=1S/C9H12N2/c1-4-5-9-8(3)10-6-7(2)11-9/h4-6H,1-3H3/b5-4+
InchiKey:	UPGLIDCBHZSEJE-SNAWJCMRSA-N
Formula:	C9H12N2
SMILES:	CC=Cc1nc(C)cnc1C
Mol. weight [g/mol]:	148.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.127		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
rinpola	1243.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502671&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
rinpola:	Non-polar retention indices

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