

2-ethenyl-3,6-dimethylpyrazine

Other names:	2,5-dimethyl-3-vinylpyrazine
Inchi:	InChI=1S/C8H10N2/c1-4-8-7(3)9-5-6(2)10-8/h4-5H,1H2,2-3H3
InchiKey:	JLPZQZIYSREPPU-UHFFFAOYSA-N
Formula:	C8H10N2
SMILES:	<chem>C=Cc1nc(C)cnc1C</chem>
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.736		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1535.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R179038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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