

pyrazine, 2-Ethyl, 6-vinyl

Other names:	6-ethyl-2-vinylpyrazine
Inchi:	InChI=1S/C8H10N2/c1-3-7-5-9-6-8(4-2)10-7/h3,5-6H,1,4H2,2H3
InchiKey:	QKJPBHPFIVOPSX-UHFFFAOYSA-N
Formula:	C8H10N2
SMILES:	C=Cc1cncc(CC)n1
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.682		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R219780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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<https://www.chemeo.com/cid/35-594-4/pyrazine-2-Ethyl-6-vinyl.pdf>

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