

Pyrazine, 2-methyl-6-(1-propenyl)-, (E)-

Other names:	Pyrazine, 2-methyl-6-propenyl-, (E)- 2-Methyl-6-[(1E)-1-propenyl]pyrazine 2-Methyl-6-(1-propenyl) pyrazine, trans (E)-2-Methyl-6-(1-propenyl)pyrazine 2-Methyl-6-(trans-1-propenyl)pyrazine 2-Methyl-6-[(E)-1-propenyl]pyrazine
Inchi:	InChI=1S/C8H10N2/c1-3-4-8-6-9-5-7(2)10-8/h3-6H,1-2H3/b4-3+
InchiKey:	NOBVHXZAVPKZQU-ONEGZZNKSA-N
Formula:	C8H10N2
SMILES:	CC=Cc1cncc(C)n1
Mol. weight [g/mol]:	134.18
CAS:	18217-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	1.818		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18217817&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
ripol:	Polar retention indices

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