Pyrazine, 2-methyl-5-(1-propenyl)-, (E)-

Other names:	Pyrazine, 2-methyl-5-propenyl-, (E)-
	2-Methyl-5-[(1E)-1-propenyl]pyrazine
	2-Methyl-5-(1-propenyl) pyrazine, trans
	2-methyl-5-((E)-1-propenyl)-pyrazine
	(E)-5-methyl-2-(1-propenyl) pyrazine
Inchi:	InChI=1S/C8H10N2/c1-3-4-8-6-9-7(2)5-10-8/h3-6H,1-2H3/b4-3+
InchiKey:	KFZIJPOISUVMAW-ONEGZZNKSA-N
Formula:	C8H10N2
SMILES:	CC=Cc1cnc(C)cn1
Mol. weight [g/mol]:	134.18
CAS:	18217-82-8

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	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1635.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18217828&Units=SI

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