Pyrazine, 2,3-dimethyl-5-(1-propenyl)-, (Z)-

Other names:	2,3-Dimethyl-5-(Z-1-propenyl)-pyrazine
	2,3-Dimethyl-5-[(1Z)-1-propenyl]pyrazine
Inchi:	InChI=1S/C9H12N2/c1-4-5-9-6-10-7(2)8(3)11-9/h4-6H,1-3H3/b5-4+
InchiKey:	BNYRAFHQRSHWGQ-SNAWJCMRSA-N
Formula:	C9H12N2
SMILES:	CC=Cc1cnc(C)c(C)n1
Mol. weight [g/mol]:	148.21
CAS:	55138-72-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.127		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
rinpol	1247.00		NIST Webbook
ripol	1702.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55138722&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