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

Other names: 2-Allyl-5-methylpyrazine
Inchi: InChI=1S/C8H10N2/c1-3-4-8-6-9-7(2)5-10-8/h3,5-6H,1,4H2,2H3
InchiKey: JCZDTOUEQCNMKI-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: C=CCc1cnc(C)cn1
Mol. weight [g/mol]: 134.18
CAS: 55138-63-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.514		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1074.00		NIST Webbook
rinpol	1090.00		NIST Webbook
ripol	1535.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55138631&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
ripol: Polar retention indices