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

Other names: 2-Methyl-6-(Z-1-propenyl)pyrazine
2-Methyl-6-[(1Z)-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-ARJAWSKDSA-N
Formula: C8H10N2
SMILES: CC=Cc1cncc(C)n1
Mol. weight [g/mol]: 134.18
CAS: 55138-67-5

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	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1628.00		NIST Webbook

Sources

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=C55138675&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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