

2-ethenyl-3-ethyl-5-methylpyrazine

Other names: Pyrazine, 2-ethenyl-3-ethyl-5-methyl
Inchi: InChI=1S/C9H12N2/c1-4-8-9(5-2)11-7(3)6-10-8/h4,6H,1,5H2,2-3H3
InchiKey: YSQNQOKRWIKETP-UHFFFAOYSA-N
Formula: C9H12N2
SMILES: C=Cc1ncc(C)nc1CC
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.990		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
rinpol	1172.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1585.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R237728&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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