2-ethenyl-3,6-dimethylpyrazine

Other names: 2,5-dimethyl-3-vinylpyrazine
Inchi: InChI=1S/C8H10N2/c1-4-8-7(3)9-5-6(2)10-8/h4-5H,1H2,2-3H3
InchiKey: JLPZQZIYSREPPU-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: C=Cc1nc(C)cnc1C
Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.736		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1535.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R179038&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