E-2-propenyl-3,5-dimethylpyrazine

Inchi: InChI=1S/C9H12N2/c1-4-5-9-8(3)11-7(2)6-10-9/h4-6H,1-3H3/b5-4+
InchiKey: NDDMVJXHROIJBV-SNAWJCMRSA-N
Formula: C9H12N2
SMILES: CC=Cc1ncc(C)nc1C
Mol. weight [g/mol]: 148.21

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	1236.00		NIST Webbook
ripol	1696.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R500026&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