Pyrazine, 2,3-dimethyl-5-(1-methylethyl)

Other names: 2,3-dimethyl-5-isopropylpyrazine
Inchi: InChI=1S/C9H14N2/c1-6(2)9-5-10-7(3)8(4)11-9/h5-6H,1-4H3
InchiKey: JTIYGJBEUZEJAB-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: Cc1ncc(C(C)C)nc1C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.217		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1454.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38242&Units=SI

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