

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:	<chem>Cc1ncc(C(C)C)nc1C</chem>
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/ci990307I
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

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