2-isobutyl-5-methylpyrazine

Other names:	Pyrazine, 5-methyl-2-(2-methylpropyl)
	2-Methyl-5-isobutylpyrazine
Inchi:	InChI=1S/C9H14N2/c1-7(2)4-9-6-10-8(3)5-11-9/h5-7H,4H2,1-3H3
InchiKey:	IZEBGMNIMQBAJR-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	Cc1cnc(CC(C)C)cn1
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.984		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
ripol	1492.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1490.00		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=R266390&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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