2-chloro-5-isobutyl-3-methylpyrazine

Other names:	Pyrazine, 2-chloro-3-methyl-5-(2-methylpropyl)
Inchi:	InChI=1S/C9H13ClN2/c1-6(2)4-8-5-11-9(10)7(3)12-8/h5-6H,4H2,1-3H3
InchiKey:	BLAZRQIWPGECMI-UHFFFAOYSA-N
Formula:	C9H13ClN2
SMILES:	Cc1nc(CC(C)C)cnc1Cl
Mol. weight [g/mol]:	184.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.637		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	1600.00		NIST Webbook

Sources

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=R38292&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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