

Pyrazine, 2-chloro-3-methyl-5-(1-methylbutyl)

Inchi:	InChI=1S/C10H15ClN2/c1-4-5-7(2)9-6-12-10(11)8(3)13-9/h6-7H,4-5H2,1-3H3
InchiKey:	QZQARCSNJYEEQU-UHFFFAOYSA-N
Formula:	C10H15ClN2
SMILES:	CCCC(C)c1cnc(Cl)c(C)n1
Mol. weight [g/mol]:	198.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	3.342		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
ripol	1577.00		NIST Webbook
ripol	1577.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R217497&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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<https://www.cheméo.com/cid/90-960-6/Pyrazine-2-chloro-3-methyl-5-1-methylbutyl.pdf>

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