

Pyrazine, 2-chloro-3-(2-methylpropyl)-

Other names:	2-chloro-3-isobutylpyrazine
Inchi:	InChI=1S/C8H11ClN2/c1-6(2)5-7-8(9)11-4-3-10-7/h3-4,6H,5H2,1-2H3
InchiKey:	ZWVNFQUBQJXJOP-UHFFFAOYSA-N
Formula:	C8H11ClN2
SMILES:	CC(C)Cc1nccnc1Cl
Mol. weight [g/mol]:	170.64
CAS:	57674-17-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	2.329		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
rinpol	1187.00		NIST Webbook
ripol	1575.00		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=C57674176&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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