

2-Chloro-3-(3-methyl-2-pyrazinylmethyl)pyrazine

Inchi:	InChI=1S/C10H9CIN4/c1-7-8(13-3-2-12-7)6-9-10(11)15-5-4-14-9/h2-5H,6H2,1H3
InchiKey:	FGZJOKPIMZTLJT-UHFFFAOYSA-N
Formula:	C10H9CIN4
SMILES:	Cc1nccnc1Cc1nccnc1Cl
Mol. weight [g/mol]:	220.66
CAS:	93409-03-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	1.819		Crippen Method
mcvol	156.400	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C93409031&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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