

5-Isopropyl-3-methyl-2-(methylthio)pyrazine

Other names:	Pyrazine, 3-methyl-5-(1-methylethyl)-2-(methylthio)
Inchi:	InChI=1S/C9H14N2S/c1-6(2)8-5-10-9(12-4)7(3)11-8/h5-6H,1-4H3
InchiKey:	KDTCGKNUJMPSDM-UHFFFAOYSA-N
Formula:	C9H14N2S
SMILES:	CSc1ncc(C(C)C)nc1C
Mol. weight [g/mol]:	182.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	2.630		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
rinpol	1362.00		NIST Webbook
ripol	1737.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/19-911-9/5-Isopropyl-3-methyl-2-methylthio-pyrazine.pdf>

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