

Pyrazine, 3-methoxy-2-(2-methylbutyl)

Other names:	Pyrazine, 2-methoxy-3-(2-methylbutyl)
Inchi:	InChI=1S/C10H16N2O/c1-4-8(2)7-9-10(13-3)12-6-5-11-9/h5-6,8H,4,7H2,1-3H3
InchiKey:	WRBWGXGWEBJRYDC-UHFFFAOYSA-N
Formula:	C10H16N2O
SMILES:	CCC(C)Cc1nccnc1OC
Mol. weight [g/mol]:	180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.074		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1267.00		NIST Webbook
ripol	1609.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R43716&Units=SI

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/33-513-5/Pyrazine-3-methoxy-2-2-methylbutyl.pdf>

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