

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

Other names:	2-methyl-5-isopentylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-8(2)4-5-10-7-11-9(3)6-12-10/h6-8H,4-5H2,1-3H3
InchiKey:	NLWRBWNTZWAQLB-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	Cc1cnc(CCC(C)C)cn1
Mol. weight [g/mol]:	164.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.374		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpola	1228.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R221500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices

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<https://www.chemeo.com/cid/19-686-0/Pyrazine-2-methyl-5-3-methylbutyl.pdf>

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