

2-(3-Methylbutyl)-3,5-dimethylpyrazine

Other names:	2,6-Dimethyl-3-isopentylpyrazine 2-Isopentyl-3,5-dimethylpyrazine
Inchi:	InChI=1S/C11H18N2/c1-8(2)5-6-11-10(4)13-9(3)7-12-11/h7-8H,5-6H2,1-4H3
InchiKey:	ZVLSVDOZUWUIJ-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	Cc1cnc(CCC(C)C)c(C)n1
Mol. weight [g/mol]:	178.27
CAS:	111150-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.682		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
ripol	1530.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1530.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111150302&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
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/78-870-0/2-3-Methylbutyl-3-5-dimethylpyrazine.pdf>

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