

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

Other names:	Pyrazine, 3-isopentyl-2,5-dimethyl- 2,5-Dimethyl-3-isoamylpyrazine 2,5-Dimethyl-3-isopentylpyrazine 3-Isoamyl-2,5-dimethylpyrazine 3-Isopentyl-2,5-dimethyl-pyrazine 2-(3-Methylbutyl)-3,6-dimethylpyrazine 2,5-Dimethyl-3(3'-methylbutyl)pyrazine 2,5-dimethyl-3-(3-methylbutyl)pyrazine 2-isopentyl-3,6-dimethylpyrazine
Inchi:	InChI=1S/C11H18N2/c1-8(2)5-6-11-10(4)12-7-9(3)13-11/h7-8H,5-6H2,1-4H3
InchiKey:	WWAYKGYKYHEINT-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	Cc1cnc(C)c(CCC(C)C)n1
Mol. weight [g/mol]:	178.27
CAS:	18433-98-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.682		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1323.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1310.00		NIST Webbook
ripol	1666.00		NIST Webbook

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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18433982&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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