

# 2-(2-Methylpropyl)-3,5,6-trimethylpyrazine

<b>Other names:</b>	Pyrazine, 3,5,6-trimethyl-2-isobutyl trimethylisobutylpyrazine 2-Isobutyl-3,5,6-trimethylpyrazine
<b>Inchi:</b>	InChI=1S/C11H18N2/c1-7(2)6-11-10(5)12-8(3)9(4)13-11/h7H,6H2,1-5H3
<b>InchiKey:</b>	CMCOFWHSAGPVSF-UHFFFAOYSA-N
<b>Formula:</b>	C11H18N2
<b>SMILES:</b>	Cc1nc(C)c(CC(C)C)nc1C
<b>Mol. weight [g/mol]:</b>	178.27
<b>CAS:</b>	46187-37-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	2.600		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1556.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C46187375&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C46187375&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## 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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