

# Pyrazine, 2-butyl-3,5-dimethyl-

<b>Other names:</b>	3,5-Dimethyl-2-butylpyrazine 3-Butyl-2,6-dimethylpyrazine 2-butyl-3,5-dimethylpyrazine
<b>Inchi:</b>	InChI=1S/C10H16N2/c1-4-5-6-10-9(3)12-8(2)7-11-10/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	CSGGOEENSRAPU-UHFFFAOYSA-N
<b>Formula:</b>	C10H16N2
<b>SMILES:</b>	CCCCc1ncc(C)nc1C
<b>Mol. weight [g/mol]:</b>	164.25
<b>CAS:</b>	50888-63-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.436		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1196.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1583.00		NIST Webbook

## Sources

<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>
<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=C50888636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50888636&amp;Units=SI</a>

# Legend

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

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