

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

<b>Other names:</b>	2,5-Dimethyl-3-butylpyrazine 3-Butyl-2,5-dimethylpyrazine 2-Butyl-3,6-dimethylpyrazine
<b>Inchi:</b>	InChI=1S/C10H16N2/c1-4-5-6-10-9(3)11-7-8(2)12-10/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	UWJKKFNWVRAFPM-UHFFFAOYSA-N
<b>Formula:</b>	C10H16N2
<b>SMILES:</b>	CCCCc1nc(C)cnc1C
<b>Mol. weight [g/mol]:</b>	164.25
<b>CAS:</b>	40790-29-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.436		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
ripol	1263.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1487.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C40790292&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40790292&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## 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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