

Pyrazine, 2,3-dimethyl-5-(1-methylpropyl)-

Other names:	Pyrazine, 5-sec-butyl-2,3-dimethyl- 2,3-Dimethyl-5-sec-butylpyrazine 5-sec-Butyl-2,3-dimethylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-5-7(2)10-6-11-8(3)9(4)12-10/h6-7H,5H2,1-4H3
InchiKey:	ZTPIKPFNCVSISS-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	CCC(C)c1cnc(C)c(C)n1
Mol. weight [g/mol]:	164.25
CAS:	32263-00-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.607		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
ripol	1194.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32263006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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<https://www.chemeo.com/cid/19-495-2/Pyrazine-2-3-dimethyl-5-1-methylpropyl.pdf>

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