

2-Isobutyl-3-methylpyrazine

Other names:	Pyrazine, 2-methyl-3-(2-methylpropyl)- 2-Methyl-3-(2-methylpropyl)pyrazine 3-Methyl-2-isobutyl pyrazine
Inchi:	InChI=1S/C9H14N2/c1-7(2)6-9-8(3)10-4-5-11-9/h4-5,7H,6H2,1-3H3
InchiKey:	ZHMIODDNZRIENW-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	Cc1nccnc1CC(C)C
Mol. weight [g/mol]:	150.22
CAS:	13925-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.984		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1114.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	1490.00		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=C13925069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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