

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

Other names:	Pyrazine, 3-isobutyl-2,5-dimethyl- 2,5-Dimethyl-3-isobutylpyrazine 3-Isobutyl-2,5-dimethylpyrazine 2,5-Dimethyl-3-(2-methylpropyl)pyrazine 2,5-Dimethyl-6-isobutylpyrazine 3,6-Dimethyl-2-isobutylpyrazine
Inchi:	InChI=1S/C10H16N2/c1-7(2)5-10-9(4)11-6-8(3)12-10/h6-7H,5H2,1-4H3
InchiKey:	KEJJOEQXAEQCAKT-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	<chem>Cc1cnc(C)c(CC(C)C)n1</chem>
Mol. weight [g/mol]:	164.25
CAS:	32736-94-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.292		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1184.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1549.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C32736940&Units=SI>

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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