

3,5-Dimethyl-2-isobutylpyrazine

Other names:	2-(2-Methylpropyl)-3,5-dimethylpyrazine 2,6-Dimethyl-3-(2-methylpropyl)pyrazine 2,6-Dimethyl-5-isobutylpyrazine 3,5-Dimethyl-2-(2-methylpropyl)pyrazine Pyrazine, 3,5-dimethyl-2-(2-methylpropyl)-
Inchi:	InChI=1S/C10H16N2/c1-7(2)5-10-9(4)12-8(3)6-11-10/h6-7H,5H2,1-4H3
InchiKey:	PBBZXNLEMPGGCH-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	<chem>Cc1cnc(CC(C)C)c(C)n1</chem>
Mol. weight [g/mol]:	164.25
CAS:	70303-42-3

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	1211.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1209.00		NIST Webbook
ripol	1549.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70303423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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