

Pyrazine, 2-ethoxy-3-methyl-5-(2-methylpropyl)

Other names:	2-Ethoxy-5-isobutyl-3-methylpyrazine
Inchi:	InChI=1S/C11H18N2O/c1-5-14-11-9(4)13-10(7-12-11)6-8(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	VDQQWQBPRGKQBH-UHFFFAOYSA-N
Formula:	C11H18N2O
SMILES:	CCOc1ncc(CC(C)C)nc1C
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.382		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpola	1314.00		NIST Webbook
ripola	1584.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices

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