5-methyl-3-isopropyl-2-methoxypyrazine

Other names: 3-Isopropyl-2-methoxy-5-methylpyrazine
Inchi: InChI=1S/C9H14N2O/c1-6(2)8-9(12-4)10-5-7(3)11-8/h5-6H,1-4H3
InchiKey: NCKFIUKGRGDXBF-UHFFFAOYSA-N
Formula: C9H14N2O
SMILES: COc1ncc(C)nc1C(C)C
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.917		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1149.00		NIST Webbook
ripol	1440.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R325929&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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