

Pyrazine, 2-methoxy-3-methyl-5-(1-methylethyl)

Other names: 5-isopropyl-3-methyl-2-methoxypyrazine
Inchi: InChI=1S/C9H14N2O/c1-6(2)8-5-10-9(12-4)7(3)11-8/h5-6H,1-4H3
InchiKey: WVRCUMDMHNIPJX-UHFFFAOYSA-N
Formula: C9H14N2O
SMILES: COc1ncc(C(C)C)nc1C
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	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1467.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R38630&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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