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

Other names: 5-isobutyl-3-methyl-2-methoxypyrazine
Inchi: InChI=1S/C10H16N2O/c1-7(2)5-9-6-11-10(13-4)8(3)12-9/h6-7H,5H2,1-4H3
InchiKey: RSRBELMBYIBNLC-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: COc1ncc(CC(C)C)nc1C
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	1.992		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1257.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1556.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38591&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