3-Methyl-2-methoxy-5-(2-methylbutyl)pyrazine

Other names: Pyrazine, 2-methoxy-3-methyl-5-(2-methylbutyl)
Inchi: InChI=1S/C11H18N2O/c1-5-8(2)6-10-7-12-11(14-4)9(3)13-10/h7-8H,5-6H2,1-4H3
InchiKey: SMSDNXXXQGQISN-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: CCC(C)Cc1cnc(OC)c(C)n1
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
rinpol	1362.00		NIST Webbook
rinpol	1362.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1664.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38505&Units=SI
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

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