Pyrazine, 2-(3-methylpentyl)-3-methoxy

Inchi: InChI=1S/C11H18N2O/c1-4-9(2)5-6-10-11(14-3)13-8-7-12-10/h7-9H,4-6H2,1-3H3
InchiKey: XCGYYKCDQJOWDP-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: CCC(C)CCc1nccnc1OC
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.464		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R43364&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

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