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

Inchi: InChI=1S/C11H18N2O/c1-4-5-9(2)8-10-11(14-3)13-7-6-12-10/h6-7,9H,4-5,8H2,1-3H3
InchiKey: DPDAVCMJBIIPLV-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: CCCC(C)Cc1nccnc1OC
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
ripol	1677.00		NIST Webbook
ripol	1677.00		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=R218029&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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