Pyrazine, 2-(4-pentenyl)-3-methoxy

Other names: Pyrazine, 2-methoxy-3-(4-pentenyl)
Inchi: InChI=1S/C10H14N2O/c1-3-4-5-6-9-10(13-2)12-8-7-11-9/h3,7-8H,1,4-6H2,2H3
InchiKey: ACVNEKTUKYFZNP-UHFFFAOYSA-N
Formula: C10H14N2O
SMILES: C=CCCCc1nccnc1OC
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	1.994		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
rinpol	1302.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook

Sources

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=R43485&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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