Pyrazine, 2-hexyl-3-methoxy

Inchi: InChI=1S/C11H18N2O/c1-3-4-5-6-7-10-11(14-2)13-9-8-12-10/h8-9H,3-7H2,1-2H3
InchiKey: GMDSOYPKWWYSJC-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: CCCCCCc1nccnc1OC
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.608		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1767.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R43453&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