2-methyl-5-(2-methylbutyl)-3-octylpyrazine

Other names: Pyrazine, 2-methyl-5-(2-methylbutyl)-3-octyl
Inchi: InChI=1S/C18H32N2/c1-5-7-8-9-10-11-12-18-16(4)19-14-17(20-18)13-15(3)6-2/h14-15H
InchiKey: MFZVESAUFHTENP-UHFFFAOYSA-N
Formula: C18H32N2
SMILES: CCCCCCCCc1nc(CC(C)CC)cnc1C
Mol. weight [g/mol]: 276.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	5.277		Crippen Method
mcvol	260.680	ml/mol	McGowan Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R38434&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