Pyrazine, 2-isopentyl-3-methoxy

Other names: Pyrazine, 3-methoxy-2-(3-methylbutyl)
Inchi: InChI=1S/C10H16N2O/c1-8(2)4-5-9-10(13-3)12-7-6-11-9/h6-8H,4-5H2,1-3H3
InchiKey: TVXVTADJOKTTIV-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: COc1nccnc1CCC(C)C
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.074		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1616.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R43734&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