3-sec-Butyl-2-methoxy-5-methylpyrazine

Inchi: InChI=1S/C10H16N2O/c1-5-7(2)9-10(13-4)11-6-8(3)12-9/h6-7H,5H2,1-4H3
InchiKey: VPZHXSRAUPOUQO-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: CCC(C)c1nc(C)cnc1OC
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	2.307		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		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=R388995&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.