3-sec-Butyl-2-methoxy-6-methylpyrazine

Inchi:	InChI=1S/C10H16N2O/c1-5-7(2)9-10(13-4)12-8(3)6-11-9/h6-7H,5H2,1-4H3
InchiKey:	LXTURXRWQRUDCZ-UHFFFAOYSA-N
Formula:	C10H16N2O
SMILES:	CCC(C)c1ncc(C)nc1OC
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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389007&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

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