

2-[(3-Hydroxy-2,2,4,4-tetramethyl)cyclobutoxy]-3-methylpyrazine

Inchi:	InChI=1S/C13H20N2O2/c1-8-9(15-7-6-14-8)17-11-12(2,3)10(16)13(11,4)5/h6-7,10-11,16
InchiKey:	PHPGPEBNVOPTBL-UHFFFAOYSA-N
Formula:	C13H20N2O2
SMILES:	Cc1nccnc1OC1C(C)(C)C(O)C1(C)C
Mol. weight [g/mol]:	236.31
CAS:	116660-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	1.959		Crippen Method
mcvol	191.110	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116660390&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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