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

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/ci990307l
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