2-(1,1-Diethoxyethyl)imidazole

Inchi: InChI=1S/C9H16N2O2/c1-4-12-9(3,13-5-2)8-10-6-7-11-8/h6-7H,4-5H2,1-3H3,(H,10,11)
InchiKey: XURVJNRJSCUTKM-UHFFFAOYSA-N
Formula: C9H16N2O2
SMILES: CCOC(C)(OCC)c1ncc[nH]1
Mol. weight [g/mol]: 184.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.173		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
rinpol	1197.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R534440&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices