2-(2,2-Diethoxyethyl)imidazole

Inchi: InChI=1S/C9H16N2O2/c1-3-12-9(13-4-2)7-8-10-5-6-11-8/h5-6,9H,3-4,7H2,1-2H3,(H,10,1
InchiKey: SEPXIBIESLXLJY-UHFFFAOYSA-N
Formula: C9H16N2O2
SMILES: CCOC(Cc1ncc[nH]1)OCC
Mol. weight [g/mol]: 184.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	0.869		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
rinpol	1199.00		NIST Webbook

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=R534460&Units=SI

Legend

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