2-(4,4-Diethoxybutyl)imidazole

Inchi: InChI=1S/C11H20N2O2/c1-3-14-11(15-4-2)7-5-6-10-12-8-9-13-10/h8-9,11H,3-7H2,1-2H3
InchiKey: OFETZLLDLPPBJQ-UHFFFAOYSA-N
Formula: C11H20N2O2
SMILES: CCOC(CCCc1ncc[nH]1)OCC
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.650		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R534480&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

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