

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
rinpole	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/ci9903071
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
rinpole:	Non-polar retention indices

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