

1H-Imidazole, 2-(diethoxymethyl)-

Other names:	Imidazole-2-carboxaldehyde, diethyl acetal 2-(1,1-Diethoxymethyl)imidazole
Inchi:	InChI=1S/C8H14N2O2/c1-3-11-8(12-4-2)7-9-5-6-10-7/h5-6,8H,3-4H2,1-2H3,(H,9,10)
InchiKey:	GDYWVVQIJJWUFA-UHFFFAOYSA-N
Formula:	C8H14N2O2
SMILES:	CCOC(OCC)c1ncc[nH]1
Mol. weight [g/mol]:	170.21
CAS:	13750-84-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.999		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13750840&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
rinpol:	Non-polar retention indices

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