2-Furaldehyde diethyl acetal

Other names:	Furan, 2-(diethoxymethyl)- 2-(Diethoxymethyl)furan
Inchi:	InChI=1S/C9H14O3/c1-3-10-9(11-4-2)8-6-5-7-12-8/h5-7,9H,3-4H2,1-2H3
InchiKey:	SEILDMUKBMYIEZ-UHFFFAOYSA-N
Formula:	C9H14O3
SMILES:	CCOC(OCC)c1ccco1
Mol. weight [g/mol]:	170.21
CAS:	13529-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	2.351		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
rinpol	1078.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1453.00		NIST Webbook
tb	463.20	K	NIST Webbook
tb	464.70	K	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=C13529276&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature