

4H-3,1-benzoxazine-2,4(1h)-dione, 6,7,8-trimethoxy-n-methyl-

Inchi:	InChI=1S/C12H13NO6/c1-13-8-6(11(14)19-12(13)15)5-7(16-2)9(17-3)10(8)18-4/h5H,1-4
InchiKey:	KZJIRKYXXMCMFY-UHFFFAOYSA-N
Formula:	C12H13NO6
SMILES:	COc1cc2c(=O)oc(=O)n(C)c2c(OC)c1OC
Mol. weight [g/mol]:	267.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	0.518		Crippen Method
mcvol	181.920	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005270&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

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