2,2',4,4'-Tetramethoxydiphenylnitrogen oxide

Inchi: InChI=1S/C16H18NO5/c1-19-11-5-7-13(15(9-11)21-3)17(18)14-8-6-12(20-2)10-16(14)22
InchiKey: ISMMKENMKBOESJ-UHFFFAOYSA-N
Formula: C16H18NO5
SMILES: COc1ccc(N([O])c2ccc(OC)cc2OC)c(OC)c1
Mol. weight [g/mol]: 304.32
CAS: 3788-15-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.12		Crippen Method
logp	3.205		Crippen Method
mcvol	225.960	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	144.00 ± 11.00	kJ/mol	348.00	NIST Webbook
hsubt	144.00 ± 11.00	kJ/mol	333.00	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=C3788156&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume