PHOSPHOROTHIOIC ACID, O,O,O-TRIMETHYL ESTER

Other names:	Phosphorothioic acid, O,O,O-trimethyl ester
	HC 7900
	Methyl phosphorothioate ((MeO)3PS)
	O,O,O-Trimethyl phosphorothioate
	SD 4741
	Trimethoxyphosphine sulfide
	Trimethyl thionophosphate
	7900-HC
	(CH3O)3PS
	Trimethyl thiophosphate
	O,O,O-Trimethylester kyseliny thiofosforecne
	Trimethylthiofosfat
	O,O,O-Trimethylthiofosfat
	O,O',O''-Trimethyl thiophosphate
	o,o',o''-Trimethyl thiophosphate
Inchi:	InChI=1S/C3H9O3PS/c1-4-7(8,5-2)6-3/h1-3H3
InchiKey:	XWSLYQXUTWUIKM-UHFFFAOYSA-N
Formula:	C3H9O3PS
SMILES:	COP(=S)(OC)OC
Mol. weight [g/mol]:	156.14

Physical Properties

Property code	Value	Unit	Source
affp	883.60	kJ/mol	NIST Webbook
basg	853.90	kJ/mol	NIST Webbook
ie	9.16	eV	NIST Webbook
logp	1.150		Crippen Method
mcvol	107.550	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C152181&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume