

O,O,O-Trimethyl thiophosphate

Other names:	Phosphorothioic acid, O,O,O-trimethyl ester HC 7900 Methyl phosphorothioate ((MeO) ₃ PS) O,O,O-Trimethyl phosphorothioate SD 4741 Trimethoxyphosphine sulfide Trimethyl thionophosphate 7900-HC (CH ₃ O) ₃ PS 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
CAS:	152-18-1

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
log10ws	3.41		Crippen Method
logp	1.150		Crippen Method
mcvol	107.550	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C152181&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

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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