

Phosphorothioic acid, O,O,S-trimethyl ester

Other names:	Dimethylthiomethylphosphate HC 7901 Methyl Phosphorothioate ((meo)2(mes)po) O,O-Dimethyl S-methyl phosphorothioate 8000 BIS HC O,O,S-Trimethyl phosphorothioate Phosphorothioic acid, o,o',s-trimethyl ester
Inchi:	InChI=1S/C3H9O3PS/c1-5-7(4,6-2)8-3/h1-3H3
InchiKey:	WTUNGUOZHBRADH-UHFFFAOYSA-N
Formula:	C3H9O3PS
SMILES:	COP(=O)(OC)SC
Mol. weight [g/mol]:	156.14
CAS:	152-20-5

Physical Properties

Property code	Value	Unit	Source
ie	9.55 ± 0.10	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	1.750		Crippen Method
mcvol	107.550	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C152205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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