# Phosphorodithioic acid, O,S,S-trimethyl ester

**Other names:** O,S,S-Trimethyl phosphorodithioate
**Inchi:** InChI=1S/C3H9O2PS2/c1-5-6(4,7-2)8-3/h1-3H3
**InchiKey:** NIJIQSOYZWDHAQ-UHFFFAOYSA-N
**Formula:** C3H9O2PS2
**SMILES:** COP(=O)(SC)SC
**Mol. weight [g/mol]:** 172.21
**CAS:** 22608-53-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 9.20 ± 0.10 | eV | NIST Webbook |
| log10ws | -3.20 | | Crippen Method |
| logp | 2.467 | | Crippen Method |
| mcvol | 118.030 | ml/mol | McGowan Method |

## 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=C22608533&Units=SI

## Legend

**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume