

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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/58-124-0/Phosphorodithioic-acid-O-S-S-trimethyl-ester.pdf>

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