Phosphorodichloridothioic acid, o-(1-methylethyl) ester

Inchi: InChI=1S/C3H7Cl2OPS/c1-3(2)6-7(4,5)8/h3H,1-2H3
InchiKey: LRCCRBDJEFGERO-UHFFFAOYSA-N
Formula: C3H7Cl2OPS
SMILES: CC(C)OP(=S)(Cl)Cl
Mol. weight [g/mol]: 193.03
CAS: 19021-61-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.16		Crippen Method
logp	3.113		Crippen Method
mcvol	120.290	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19021615&Units=SI
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

Legend

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