

Phosphonothioic acid, methyl-, o,o-diisopropyl ester

Inchi:	InChI=1S/C7H17O2PS/c1-6(2)8-10(5,11)9-7(3)4/h6-7H,1-5H3
InchiKey:	WJZQSIVAHFZAQJ-UHFFFAOYSA-N
Formula:	C7H17O2PS
SMILES:	CC(C)OP(C)(=S)OC(C)C
Mol. weight [g/mol]:	196.25
CAS:	66295-45-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.59		Crippen Method
logp	2.776		Crippen Method
mcvol	158.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66295452&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

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

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