

Phosphorothiolothionic acid, o,o,s-triethyl ester

Inchi:	InChI=1S/C6H15O2PS2/c1-4-7-9(10,8-5-2)11-6-3/h4-6H2,1-3H3
InchiKey:	BZVCTTJRBWHTOF-UHFFFAOYSA-N
Formula:	C6H15O2PS2
SMILES:	CCOP(=S)(OCC)SCC
Mol. weight [g/mol]:	214.29
CAS:	2524-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.35		Crippen Method
logp	3.037		Crippen Method
mcvol	160.300	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C2524096&Units=SI

Legend

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

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