

Methylphosphonothioic acid, o,o-dipentyl ester

Inchi:	InChI=1S/C11H25O2PS/c1-4-6-8-10-12-14(3,15)13-11-9-7-5-2/h4-11H2,1-3H3
InchiKey:	RUEVNJMXKUBJFK-UHFFFAOYSA-N
Formula:	C11H25O2PS
SMILES:	CCCCCOP(C)(=S)OCCCCC
Mol. weight [g/mol]:	252.35
CAS:	91964-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.14		Crippen Method
logp	4.339		Crippen Method
mcvol	214.400	ml/mol	McGowan Method

Sources

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=C91964759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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