

Diethyl methylthiomethylphosphonate

Inchi:	InChI=1S/C6H15O3PS/c1-4-8-10(7,6-11-3)9-5-2/h4-6H2,1-3H3
InchiKey:	RAABCCZMKIIGJW-UHFFFAOYSA-N
Formula:	C6H15O3PS
SMILES:	CCOP(=O)(CSC)OCC
Mol. weight [g/mol]:	198.22
CAS:	28460-01-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	2.573		Crippen Method
mcvol	149.820	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=C28460017&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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