

Crotoxyphos

Other names:	2-Butenoic acid, 3-[(dimethoxyphosphinyloxy)-, 1-phenylethyl ester, (E)- Crotonic acid, 3-hydroxy-, «alpha»-methylbenzyl ester, dimethyl phosphate, (E)- Ciodrin Cyodrin Dimethyl 2-(«alpha»-methylbenzyloxycarbonyl)-1-methylvinyl phosphate Shell SD 4294 SD 4294 Volfazol 3-Hydroxycrotonic acid «alpha»-methylbenzyl ester dimethyl phosphate Crotoxyfos Cypona E.C. O,O-Dimethyl O-(1-methyl-2-carboxy-«alpha»-phenylethyl)vinyl phosphate Decrotox Dimethyl-cis-1-methyl-2-(1-phenylethoxycarbonyl)vinyl phosphate Dimethyl phosphate of «alpha»-methylbenzyl 3-hydroxy-cis-crotonate Duo-kill Duravos ENT 24,717 1-Methylbenzyl-3-(dimethoxyphosphinyloxo)isocrotonate «alpha»-Methyl benzyl-3-(dimethoxy-phosphinyloxy)-crotonate, trans «alpha»-Methylbenzyl 3-hydroxycrotonate dimethyl phosphate, trans- OMS 239 Pantozol 1 cis-2-(1-Phenylethoxy)carbonyl-1-methylvinyl dimethylphosphate 1-Phenylethyl 3-(dimethoxyphosphinoxyloxy)isocrotonate Crotoxyphos-trans
Inchi:	InChI=1S/C14H19O6P/c1-11(20-21(16,17-3)18-4)10-14(15)19-12(2)13-8-6-5-7-9-13/h5-1
InchiKey:	XXXSILNSXNPGKG-ZHACJKMWSA-N
Formula:	C14H19O6P
SMILES:	<chem>COP(=O)(OC)OC(C)=CC(=O)OC(C)c1ccccc1</chem>
Mol. weight [g/mol]:	314.27
CAS:	7700-17-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method

logp	3.612		Crippen Method
mvol	231.440	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook

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=C7700176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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