2-Butenoic acid, 3-[[(ethylamino)methoxyphosphinothioyl]oxy]-, 1-methylethyl ester, (E)-

Other names: (E)-1-Methylethyl 3-(((ethylamino)methoxyphosphinothioyl)oxy)-2-butenoate

(E)-1-Metiletil-3-(((etilamino)metoxifosfinotiol)oxi)-2-butenoato

(E)-3-[[(Ethylamino)methoxyphosphinothioyl]oxy]-2-butenoic acid 1-methyl-ethyl ester

(E)-O-2-Isopropoxy-carbonyl-1-methylvinyl O-methyl ethylphosphoramidothioate

1-Methylethyl (E)-3-(((ethylamino)methoxyphosphinothioyl)oxy)-2-butenoate

2-Butenoic acid, 3-(((ethylamino)methoxyphosphinothioyl)oxy)-, isopropyl ester, (E)-

Biotic

Crotonic acid, 3-hydroxy-, isopropyl ester, O-ester with O-methyl ethylphosphoramidothioate, (E)-

Deadmag

E-Propetamphos

ENT 27989

Isopropyl (2E)-3-([(ethylamino)(methoxy)phosphorothioyl]oxy)-2-butenoate

O-(1-Isopropoxycarbonyl-1-propen-2-yl)-O-methyl N-ethyl-phosphoramidothionate

OMS 1502

Propetamphos

SAN 322I

SAN 52139

Safrotin S 200

Sandoz 52139

TSAR

VEL 4283

trans-isopropyl-3-[[(ethylamino)methoxyfosfinothioyl]oxy]crotonate

Inchi: InChI=1S/C10H20NO4PS/c1-6-11-16(17,13-5)15-9(4)7-10(12)14-8(2)3/h7-8H,6H2,1-5H3

InchiKey: BZNDWPRGXNILMS-VQHVLOKHSA-N

Formula: C10H20NO4PS

SMILES: CCNP(=S)(OC)OC(C)=CC(=O)OC(C)C

Mol. weight [g/mol]: 281.31

CAS: 31218-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Aqueous Solubility Prediction Method
log10ws	-3.41		Estimated Solubility Method
logp	2.339		Crippen Method
mcvol	213.430	ml/mol	McGowan Method

rinpol	1774.00	NIST Webbook
rinpol	1779.00	NIST Webbook
rinpol	1777.00	NIST Webbook
rinpol	1777.00	NIST Webbook
rinpol	1774.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31218834&Units=SI

Legend

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