Malaoxon

Other names:
(1,4-diethoxy-1,4-dioxobutan-2-yl)sulfanyl-hydroxy-dimethoxyphosphanium
Butanedioic acid, 2-[(dimethoxyphosphinyl)thio]-, 1,4-diethyl ester
Butanedioic acid, [(dimethoxyphosphinyl)thio]-, diethyl ester
Carbethoxy malaoxon
Diethyl mercaptosuccinate S-ester with O,O-dimethyl phosphorothioate
Liromat
Malaoxone
Malathion-O-analog
Maloxon
NCI-C08628
O,O-Dimethyl S-1,2-bis(ethoxycarbonyl)ethyl phosphorothioate
O,O-Dimethyl-S-(1,2-dicarbethoxy)ethyl phosphorothioate
Oxycarbophos
Phosphorothioic acid, O,O-dimethyl ester, S-ester with 1,2-bis(ethoxycarbonyl)ethanethiol
S-(1,2-Diethoxycarbonyl)ethyl O,O-dimethyl phosphorothioate
Succinic acid, mercapto-, diethyl ester, S-ester with O,O-dimethyl phosphorothioate

Inchi: InChI=1S/C10H19O7PS/c1-5-16-9(11)7-8(10(12)17-6-2)19-18(13,14-3)15-4/h8H,5-7H2,1
InchiKey: WSORODGWGUUOBO-UHFFFAOYSA-N
Formula: C10H19O7PS
SMILES: CCOC(=O)CC(SP(=O)(OC)OC)C(=O)OCC
Mol. weight [g/mol]: 314.29
CAS: 1634-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Aqueous Solubility Prediction Method
logp	2.005		Crippen Method
mcvol	221.060	ml/mol	McGowan Method
rinpol	1838.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1634782&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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices