Phenthoate

Other names:

Benzeneacetic acid, «alpha»-[(dimethoxyphosphinothioyl)thio]-, ethyl ester
Acetic acid, mercaptophenyl-, ethyl ester, S-ester with O,O-dimethyl phosphorodithioate
Bayer 18,510
BAY 33051
Cidemul
Cidial
Dimephenthoate
Elsan
ENT 23438
ENT 27386GC
Fenthoate
L 561
Montecatini L-561
O,O-Dimethyl S-«alpha»-Ethoxycarbonylbenzyl phosphorodithioate
Pap
Papthion
Phendal
S-«alpha»-Ethoxycarbonylbenzyl dimethyl phosphorothiolothionate
S-[«alpha»-(Ethoxycarbonyl)benzyl] O,O-dimethyl phosphorodithioate
Tsidial
Acetic acid, (O,O-dimethyldithiophosphorylphenyl)-, ethyl ester
Aimsan
BAYER 18510
Dimefenthoat
Dimephenthioate
Dimethenthoate
O,O-Dimethyl S-(1-carboethoxybenzyl) dithiophosphate
O,O-Dimethyl-S-(phenylacetic acid ethyl ester) phosphorodithioate
O,O-Dimethyl S-(phenyl)(carboethoxy)methyl phosphorodithioate
(Dimethyl S-(phenylethoxycarbonylmethyl)phosphorothiolothionate)
ENT 27386
Ethyl «alpha»-((dimethoxyphosphenothioyl)thio)benzeneacetate
Ethyl O,O-dimethyl phosphorodithioylphenyl acetate
Ethyl ester of O,O-dimethyldithiophosphoryl «alpha»-phenyl acetic acid
Ethyl mercaptophenylacetate-O,O-dimethylphosphorodithioate
NSC 190978
OMS 1075
S 2940
Tanone
TH 346-1

	Phentoate
	Tagson
Inchi:	InChI=1S/C12H17O4PS2/c1-4-16-12(13)11(10-8-6-5-7-9-10)19-17(18,14-2)15-3/h5-9,11
InchiKey:	XAMUDJHXFNRLCY-UHFFFAOYSA-N
Formula:	C12H17O4PS2
SMILES:	CCOC(=O)C(SP(=S)(OC)OC)c1ccccc1
Mol. weight [g/mol]:	320.37
CAS:	2597-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.42		Crippen Method
logp	3.541		Crippen Method
mcvol	228.520	ml/mol	McGowan Method
rinpol	2038.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2073.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2010.00		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=C2597037&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