Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester

Othernames:

(dl) malathion
1,2-Di(ethoxycarbonyl)ethyl O,O-dimethyl phosphordithioate
1,2-Di(ethoxycarbonyl)ethyl O,O-dimethyl phosphorodithioate
AC 26691
American Cyanamid 4,049
Calmathion
Carbethoxy malathion
Carbetovur
Carbetox
Carbofos
Carbophos
Celthion
Chemathion
Cimexan
Cleensheen
Compound 4049
Cythion
Derbac-M
Detmol MA
Dicarboethoxyethyl O,O-dimethyl phosphorodithioate
Diethyl (dimethoxyphosphinothioylthio) butanedioate
Diethyl (dimethoxyphosphinothioylthio)succinate
Diethyl 2-(dimethoxyphosphinothioylthio)succinate
Diethyl [(dimethoxyphosphinothoiyl)thio]butanedioate
Diethyl mercaptosuccinate S-ester with O,O-dimethyl phosphorodithioate
Diethyl mercaptosuccinate, O,O-dimethyl dithiophosphate, S-ester
Diethyl mercaptosuccinate, O,O-dimethyl phosphorodithioate
Diethyl mercaptosuccinate, O,O-dimethyl thiophosphate
Diethyl mercaptosuccinic acid O,O-dimethyl phosphorodithioate
Diethyl mercaptosuccinic acid, S-ester of O,O-dimethyl phosphorodithioate
Dithiophosphate de O,O-dimethyle et de S-(1,2-dicarboethoxyethyle)
EL 4049
ENT 17,034
Emmatos
Emmatos extra
Ethiolacar
Etiol
Experimental insecticide 4049
Extermathion
Formal

Forthion
Fosfothion
Fosfotion
Fosfotion 550
Four thousand forty-nine
Fyfanon
Gammaxine
Hilthion
Hilthion 25WDP
Insecticide No. 4049
Karbofos
Kop-thion
Kypfos
Latka 4049
MLT
Malacide
Malafor
Malagran
Malakill
Malamar
Malamar 50
Malaphele
Malaphos
Malasol
Malaspray
Malataf
Malathion
Malathion E50
Malathion LV Concentrate
Malathion ULV
Malathione
Malathiozoo
Malathon
Malathyl
Malathyne
Malation
Malatol
Malatox
Maldison
Malmed
Malphos
Maltox
Maltox MLT

Mercaptosuccinic acid diethyl ester
Mercaptosuccinic acid diethyl ester, S-ester with O,O-dimethyl phosphorothioate
Mercaptothion
Mercaptotion
Moscarda
NA 2783
NCI-C00215
O,O-Dimethyl S-(1,2-dicarbethoxyethyl) dithiophosphate
O,O-Dimethyl S-(1,2-dicarbethoxyethyl) phosphorodithioate
O,O-Dimethyl S-(1,2-dicarbethoxyethyl) thiothionophosphate
O,O-Dimethyl S-1,2-di(ethoxycarbamyl)ethyl phosphorodithioate
O,O-Dimethyl S-1,2-di(ethoxycarbamyl)ethyl phosphorothioate
O,O-Dimethyl dithiophosphate diethylmercaptosuccinate
O,O-Dimethyl-S-(1,2-di(ethoxycarbonyl)ethyl) phosphorodithioate
O,O-Dimethyl-S-1,2-dikarbetoxylethylditiofosfat
O,O-Dwumetylo-S-1,2-bis(karboetoksyetylo)-dwutiofosforan
OMS 1
Oleophosphothion
Organoderm
Ortho Malathion
Ovide
Phosphothion
Prioderm
Radotion
S-(1,2-Bis(aethoxy-carbonyl)-aethyl)-O,O-dimethyl-dithiophasphat
S-(1,2-Bis(ethoxy-carbonyl)-ethyl)-O,O-dimethyl-dithiofosfaat
S-(1,2-Bis(etossi-carbonil)-etil)-O,O-dimetil-ditiofosfato
S-(1,2-Di(ethoxycarbonyl)ethyl) dimethyl phosphorothiolothionate
S-(1,2-Dicarbethoxyethyl) O,O-dimethyl phosphorodithioate
S-(1,2-Dicarbethoxyethyl) O,O-dimethyldithiophosphate
S-1,2-Bis(ethoxycarbonyl)ethyl-O,O-dimethyl thiophosphate
S-[1,2-Bis(carbethoxy)ethyl] O,O-dimethyl dithiophosphate
S-[1,2-Bis(ethoxycarbonyl)ethyl] O,O-dimethyl phosphorodithioate
SF 60
Sadofos
Sadofos 30
Sadophos
Siptox I
Staeubol-Puder
Succinic acid, mercapto-, diethyl ester, S-ester with O,O-dimethyl phosphorodithioate
Sulfo M
Sumitox
TAK

	TM-4049
	Taskil
	Vegfru malatox
	Vetiol
	Zithiol
	[(Dimethoxyphosphinothioyl)thio]butanedioic acid, diethyl ester
	diethyl 2-dimethoxyphosphinothioylsulfanylbutanedioate
Inchi:	InChI=1S/C10H19O6PS2/c1-5-15-9(11)7-8(10(12)16-6-2)19-17(18,13-3)14-4/h8H,5-7H2
InchiKey:	JXSJBGJIGXNWCI-UHFFFAOYSA-N
Formula:	C10H19O6PS2
SMILES:	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC
Mol. weight [g/mol]:	330.36
CAS:	121-75-5

Physical Properties

Property code	Value	Unit	Source
hf	-1097.83	kJ/mol	Cheméo Relay (1.0)
hvap	71.10	kJ/mol	NIST Webbook
log10ws	-3.37		Estimated Solubility Method
log10ws	-3.36		Aqueous Solubility Prediction Method
logp	2.122		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
rinpol	1965.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1922.00		NIST Webbook

rinpol	1970.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1926.00		NIST Webbook
ripol	2872.00		NIST Webbook
tb	604.05	K	Cheméo Relay (1.0)
tc	792.18	K	Cheméo Relay (1.0)
tf	275.95	K	Aqueous Solubility Prediction Method
tf	273.95 ± 0.50	K	NIST Webbook
tf	275.95 ± 0.35	K	NIST Webbook
tf	276.25 ± 0.25	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77036e+01
Coeff. B	-8.55779e+03
Temperature range (K), min.	491.37
Temperature range (K), max.	690.58

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121755&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point