Fenitrothion

Other names:

AC-47300
Accothion
Aceothion
Agria 1050
Agriya 1050
Agrothion
Akotion
American cyanamid cl-47,300
Arbogal
BAY 41831
BAY S 5660
Bayer 41831
Bayer S 5660
CL 47300
CP 47114
Cekutrothion
Cyfen
Cytel
Cyten
Dicofen
Dimethyl 3-methyl-4-nitrophenyl phosphorothionate
Dimethyl 4-nitro-m-tolyl phosphorothionate
EI 47300
ENT 25,715
Falithion
Fenitox
Fenitrotion
Folithion
Folithion ec 50
Kotion
MEP
MEP (Pesticide)
MEP (Phosphorus insecticide)
Macbar
Metathio E-50
Metathion
Metathion E-50
Metathione
Metathionine
Metathionine E-50

Metation
Metation E-50
Methylnitrophos
Mglawik F
Monsanto CP 47114
Nitrophos
Novathion
Nuvanol
O,O-DiMe O-(3-methyl-4-nitrophenyl) thiophosphate
O,O-Dimethyl O-(3-methyl-4-nitrophenyl) phosphorothioate
O,O-Dimethyl O-(3-methyl-4-nitrophenyl) thiophosphate
O,O-Dimethyl O-(4-nitro-3-methylphenyl)thiophosphate
O,O-Dimethyl O-4-nitro-m-tolyl phosphorothioate
O,O-Dimethyl O-4-nitro-m-tolyl thiophosphate
O,O-Dimethyl-(3-methyl-4-nitrophenyl) ester of phosphorothioic acid
O,O-Dimethyl-O-(3-methyl-4-nitro-phenyl)-monothiophosphate
O,O-Dimethyl-O-(3-methyl-4-nitrofenyl)-monothiofosfaat
O,O-Dimethyl-O-(4-nitro-5-methylphenyl)-thionophosphate
O,O-Dimetil-O-(3-metil-4-nitro-fenil)-monotiofosfato
O,O-Dimetil-O-(3-metil-4-nitrofenil) fosforotioato
OMS 43
Oleometathion
Oleosumifene
Ovadofos
Owadofos
Owadophos
Pennwalt C-4852
Phenitrothion
Phosphorothioic acid, O,O-dimethyl O-(3-methyl-4-nitrophenyl) ester
Phosphorothioic acid, O,O-dimethyl O-(4-nitro-m-tolyl) ester
S 112A
S 5660
S-1102A
Sumifene
Sumigran
Sumithian
Sumithion
Sumitomo S-1102A
Thiophosphate de O,O-dimethyle et de O-(3-methyl-4-nitrophenyle)
Tionfos 50 LE
Verthion
bis-Fenitrothion
dimethoxy-(3-methyl-4-nitrophenoxy)-sulfanylidenephosphorane

m-Cresol, 4-nitro-, O-ester with O,O-dimethyl phosphorothioate

Inchi: InChI=1S/C9H12NO5PS/c1-7-6-8(4-5-9(7)10(11)12)15-16(17,13-2)14-3/h4-6H,1-3H3

InchiKey: ZNOLGFHPUIJIMJ-UHFFFAOYSA-N

Formula: C9H12NO5PS

SMILES: COP(=S)(OC)Oc1ccc([N+](=O)[O-])c(C)c1

Mol. weight [g/mol]: 277.23

CAS: 122-14-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Estimated Solubility Method
log10ws	-4.15		Aqueous Solubility Prediction Method
logp	2.799		Crippen Method
mcvol	185.750	ml/mol	McGowan Method
rinpol	1922.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1954.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tf	276.55	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	78.00	kJ/mol	337.50	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=C122145&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point