Fenthion

Other names:

4-Methylmercapto-3-methylphenyl dimethyl thiophosphate
B 29493
BAY 29493
Baycid
Bayer 29493
Bayer 9007
Bayer S-1752
Baytex
Dmtp
ENT 25,540
ENT 25540
Entex
Fenthion 4E
Fenthion-methyl
Fenthione
Lebaycid
MPP
MPP (Pestiide)
Mercaptophos
NCI-C08651
O,O-Dimethyl O-(3-methyl-4-methylmercaptophenyl)phosphorothioate
O,O-Dimethyl O-(4-(methylthio)-m-tolyl) phosphorothioate
O,O-Dimethyl O-(4-methylthio-3-methylphenyl) phosphorothioate
O,O-Dimethyl O-4-(methylmercapto)-3-methylphenyl phosphorothioate
O,O-Dimethyl O-[3-methyl-4-(methylthio)phenyl]phosphorothioate
O,O-Dimethyl-O-(3-methyl-4-methylthio-fenyl)-monothiofosfaat
O,O-Dimethyl-O-(3-methyl-4-methylthio-phenyl)-thionophosphate
O,O-Dimethyl-O-(3-methyl-4-methylthiophenyl)-monothiophosphate
O,O-Dimethyl-O-4-(methylmercapto)-3-methylphenyl thiophosphate
O,O-Dimetil-O-(3-metil-4-metiltio-fenil)-monotiofosfato
O,O-dimethyl-O-[3-methyl-4-(methylthio)phenyl]thiophosphate
OMS 2
Phenthion
Phosphorothioic acid, O,O-dimethyl O-[3-methyl-4-(methylthio)phenyl] ester
Phosphorothioic acid, O,O-dimethyl O-[4-(methylthio)-m-tolyl] ester
Queletox
S 1752
Spotton
Sulfidophos
Talodex

	Thiophosphate de O,O-dimethyle et de O-(3-methyl-4-methylthiophenyle)
	Tiguvon
	m-Cresol, 4-(methylthio)-, O-ester with O,O-dimethyl phosphorothioate
Inchi:	InChI=1S/C10H15O3PS2/c1-8-7-9(5-6-10(8)16-4)13-14(15,11-2)12-3/h5-7H,1-4H3
InchiKey:	PNVJTZOFSHSLTO-UHFFFAOYSA-N
Formula:	C10H15O3PS2
SMILES:	COP(=S)(OC)Oc1ccc(SC)c(C)c1
Mol. weight [g/mol]:	278.33
CAS:	55-38-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Aqueous Solubility Prediction Method
log10ws	-4.57		Estimated Solubility Method
logp	3.613		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
rinpol	2009.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1957.00		NIST Webbook
ripol	2944.00		NIST Webbook
tf	280.40	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	75.60	kJ/mol	333.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.85432e+01
Coeff. B	-9.08968e+03
Temperature range (K), min.	497.91
Temperature range (K), max.	686.96

Sources

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=C55389&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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