Disulfoton

Other names:

Bay 19639
Bayer 19639
Di-Syston
Di-Syston G
Dimaz
Disipton
Disulfaton
Disystox
Dithiodemeton
Dithiophosphate de O,O-diethyle et de S-(2-ethylthio-ethyle)
Dithiosystox
Dution
ENT 23,437
ENT-23437
Ekatin TD
Ethyl thiometon
Ethylthiometon B
Frumin
Frumin AL
Frumin G
Glebofos
Insyst-D
M 74
M 74 (Pesticide)
NA 2783
O,O-Diaethyl-S-(2-aethylthio-aethyl)-dithiophosphat
O,O-Diaethyl-S-(3-thia-pentyl)-dithiophosphat
O,O-Diethyl 2-ethylthioethyl phosphorodithioate
O,O-Diethyl S-(2-eththioethyl) phosphorodithioate
O,O-Diethyl S-(2-eththioethyl) thiothionophosphate
O,O-Diethyl S-(2-ethylmercaptoethyl) dithiophosphate
O,O-Diethyl S-[2-(Ethylthio)ethyl] dithiophosphate
O,O-Diethyl S-[2-(ethylthio)ethyl] phosphorodithioate
O,O-Diethyl-S-(2-ethylthio-ethyl)-dithiofosfaat
O,O-Dietil-S-(2-etiltio-etil)-ditiofosfato
O,O-Ethyl S-2(ethylthio)ethyl phosphorodithioate
Phosphonodithioic acid, O,O-diethyl S-[2-(ethylthio)ethyl] ester
Phosphorodithioic acid, O,O-diethyl S-[2-(ethylthio)ethyl] ester
Phosphorodithionic acid, S-2-(ethylthio)ethyl-O,O-diethyl ester
RCRA Waste number P039

	S 276
	S-2-(Ethylthio)ethyl O,O-diethyl ester of phosphorodithioic acid
	Solvigran
	Solvirex
	Thiodemeton
	Thiodemetron
	VUagT 1-4
	VUagT 1964
Inchi:	InChI=1S/C8H19O2PS3/c1-4-9-11(12,10-5-2)14-8-7-13-6-3/h4-8H2,1-3H3
InchiKey:	DOFZAZXDOSGAJZ-UHFFFAOYSA-N
Formula:	C8H19O2PS3
SMILES:	CCOP(=S)(OCC)SCCSCC
Mol. weight [g/mol]:	274.40
CAS:	298-04-4

Physical Properties

Property code	Value	Unit	Source
hvap	76.70	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-4.23		Estimated Solubility Method
log10ws	-4.23		Aqueous Solubility Prediction Method
logp	3.770		Crippen Method
mcvol	204.830	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1753.00		NIST Webbook
ripol	2480.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24247e+01
Coeff. B	-1.01786e+04
Coeff. C	1.49000e+01
Temperature range (K), min.	444.90
Temperature range (K), max.	579.88

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C298044&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
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

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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