Phosphoric acid, diethyl 4-nitrophenyl ester

Other names:

Chinorta
Chinorto
Diaethyl-p-nitrophenylphosphorsaeureester
Diethyl 4-nitrophenyl phosphate
Diethyl paraoxon
Diethyl-p-nitrofenyl ester kyseliny fosforecne
E 600
E 600 (Pesticide)
ENT 16,087
Ester 25
Ethyl Paraoxan
Ethyl p-nitrophenyl ethylphosphate
Ethyl paraoxon
Eticol
Fosfakol
HC 2072
Mintaco
Mintacol
Miotisal
Miotisal A
NSC 404110
O,O'Diaethyl-p-nitrophenylphosphat
O,O-Diethyl O-p-nitrophenyl phosphate
O,O-Diethyl Phosphoric acid, O-(p-nitrophenyl) ester
O,O-Dietyl-O-p-nitrofenylfosfat
O,O-diethyl-O-(4-nitrophenyl) phosphate
Oxyparathion
Paraoxon
Paraoxon-ethyl
Paraoxone
Parathion O-analog
Parathion ethyl oxon
Parathion oxon
Paroxan
Pestox 101
Phenol, p-nitro-, ester with diethyl phosphate
Phosphachole
Phosphacol
Phosphakol
Phosphonothioic acid, diethylparanitrophenyl ester

	Phosphoric acid, diethyl p-nitrophenyl ester
	Rcra waste number P041
	Soluglacit
	Soluglaucit
	Ts 219
	diethyl (4-nitrophenyl) phosphate
	p-Nitrophenyl diethyl phosphate
Inchi:	InChI=1S/C10H14NO6P/c1-3-15-18(14,16-4-2)17-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2
InchiKey:	WYMSBXTXOHUIGT-UHFFFAOYSA-N
Formula:	C10H14NO6P
SMILES:	CCOP(=O)(OCC)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	275.20

Physical Properties

Property code	Value	Unit	Source
hf	-675.65	kJ/mol	Cheméo Relay (1.0)
hvap	92.30	kJ/mol	Cheméo Relay (1.0)
ie	9.49	eV	Cheméo Relay (1.0)
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	3.155		Crippen Method
mcvol	189.360	ml/mol	McGowan Method
rinpol	1895.00		NIST Webbook
rinpol	1880.00		NIST Webbook
ripol	2838.00		NIST Webbook
ripol	2838.00		NIST Webbook
tb	604.68	K	Cheméo Relay (1.0)
tf	297.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	87.90	kJ/mol	347.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C311455&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point