

Diethyl p-nitrophenyl phosphate

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 4-nitrophenyl ester
Phosphoric acid, diethyl p-nitrophenyl ester
Rcra waste number P041
Soluglacid
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]: 275.19
CAS: 311-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	3.155		Crippen Method
mcvol	189.360	ml/mol	McGowan Method
ripol	1880.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	2838.00		NIST Webbook
ripol	2838.00		NIST Webbook

Temperature Dependent Properties

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

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C311455&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

ripol: Polar retention indices

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