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APPENDIX 1
ROBUST SUMMARIES

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IUCLID

Data Set

Existing Chemical	:	ID: 116265-68-0
Producer related part		
Company	:	Epona Associates, LLC
Creation date	:	12.12.2005
Substance related part		
Company	:	Epona Associates, LLC
Creation date	:	12.12.2005
Status	:	
Memo	:	Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol
Printing date	:	21.12.2005
Revision date	:	
Date of last update	:	20.12.2005
Number of pages	:	10
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 187 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Melting Pt (deg C): 187.09 (Mean or Weighted MP)
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

2.2 BOILING POINT

Value	:	= 484 °C at
Decomposition	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Boiling Pt (deg C): 484.31 (Adapted Stein & Brown method)
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

2.4 VAPOUR PRESSURE

Value	:	= 1.3 - 13.4 hPa at °C
Decomposition	:	
Method	:	other (measured)
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-

hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (2) valid with restrictions
Internal company data

Flag : Critical study for SIDS endpoint

20.12.2005 (1)

Value : = .0000000000017 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)

Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Result : VP(mm Hg, 25 deg C): 1.28E-012 (Modified Grain method)

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (3) invalid
Value obtained using modeling is in disagreement with actual data

20.12.2005 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -1.56 at 25 °C
pH value :
Method : other (calculated)
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.67 estimate)

Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Result : Log Kow (KOWWIN v1.67 estimate) = -1.56

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (2) valid with restrictions
Value obtained using modeling

Flag : Critical study for SIDS endpoint

20.12.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	42610 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Water Solubility Estimate from Log Kow (WSKOW v1.41): Water Solubility at 25 deg C (mg/L): 4.261e+004 log Kow used: -1.56 (estimated) no-melting pt equation used
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Water Solubility at 25 deg C (mg/L): 4.261e+004
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Insoluble
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	
Conc. of sensitizer	:	
Rate constant	:	= .0000000002 cm^3/(molecule*sec)
Degradation	:	50 % after .1 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 200.6758 E-12 cm3/molecule-sec Half-Life = 0.053 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 0.640 Hrs Ozone Reaction: No Ozone Reaction Estimation
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Hydrolyzes slowly
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions

Internal company data

Flag : Critical study for SIDS endpoint
20.12.2005 (1)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: estimated
Year : 2005

Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Result :

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	7.64e-006	1.28	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6e+003	0

Persistence Time: 789 hr

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (2) valid with restrictions
Value obtained using modeling

Flag : Critical study for SIDS endpoint
12.12.2005 (2)

3.5 BIODEGRADATION

4. Ecotoxicity

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 2 mg/l
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2000 - mg/kg bw
Species	:	rabbit
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data

20.12.2005 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

(1) Crompton (2003) Material Safety Data Sheet, Weston 430. Revision 1.2; 10/15/2003

(2) EPI SUMMARY (v3.11)

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APPENDIX 2
EPIWIN RESULTS

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SMILES : OC(COCC(OP(OC(COCC(O)C)C)OCC(OC(CO)C)C)C)C
CHEM   : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethyl
         ethoxy)methylethoxy]tetramethyl-
CAS NUM: 036788-39-3
MOL FOR: C18 H39 O9 P1
MOL WT : 430.48
------------------------------ EPI SUMMARY (v3.11) -------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   9.1
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  -1.56

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  484.31  (Adapted Stein & Brown method)
    Melting Pt (deg C):  187.09  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  1.28E-012  (Modified Grain method)

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  4.261e+004
       log Kow used: -1.56 (estimated)
       no-melting pt equation used

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  1.1011e+005 mg/L

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Neutral Organics

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :   2.52E-017  atm-m3/mole
   Group Method:   Incomplete
 Henrys LC [VP/WSol estimate using EPI values]:  1.210E-004 atm-m3/mole

 Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model         :  -0.0233
    Non-Linear Model     :   0.0000
 Expert Survey Biodegradation Results:
    Ultimate Survey Model:   2.7018  (weeks-months)
    Primary Survey Model :   3.5858  (days-weeks  )
 Readily Biodegradable Probability (MITI Model):
    Linear Model         :  -0.0858
    Non-Linear Model     :   0.0060

 Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
   Hydroxyl Radicals Reaction:
      OVERALL OH Rate Constant = 200.6758 E-12 cm3/molecule-sec
      Half-Life =     0.053 Days (12-hr day; 1.5E6 OH/cm3)
      Half-Life =     0.640 Hrs
   Ozone Reaction:
      No Ozone Reaction Estimation
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Soil Adsorption Coefficient (PCKOCWIN v1.66):
     Koc    :  10
     Log Koc:  1.000

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
   Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
   Log BCF =  0.500  (BCF = 3.162)
      log Kow used: -1.56 (estimated)

Volatilization from Water:
   Henry LC:  2.52E-017 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River:  4.82E+013  hours   (2.009E+012 days)
   Half-Life from Model Lake : 5.259E+014  hours   (2.191E+013 days)

Removal In Wastewater Treatment (recommended maximum 99%):
   Total removal:                1.85  percent
   Total biodegradation:         0.09  percent
   Total sludge adsorption:      1.75  percent
   Total to Air:                 0.00  percent

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)       (kg/hr)
  Air       4.36e-010      1.28         1000
  Water     49.8           900          1000
  Soil      50.1           900          1000
  Sediment  0.0918         3.6e+003     0
    Persistence Time: 789 hr
```