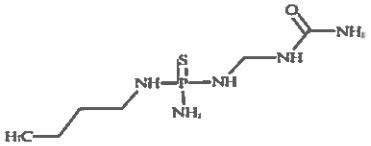
CAS Number:
SMILES : CCCCNP(=S)(N)NCNC(=O)N
CHEM : K32A
MOL FOR: C6 H18 N5 O1 P1 S1
MOL WT : 239.28

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -1.69

Boiling Pt, Melting Pt, Vapor Pressure Estimation:
Boiling Pt (deg C): 392.81 (Adapted Stein &
Melting Pt (deg C): 85.17 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 3.29E-006 (Modified Grain method)
VP (Pa, 25 deg C) : 0.000439 (Modified Grain method)
Subcooled liquid VP: 1.24E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00166 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 3.711e+004
log Kow used: -1.69 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 2.5996e+005 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Substituted Ureas

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 1.14E-015 atm-m3/mole (1.16E-010 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.791E-011 atm-m3/mole (2.828E-006 Pa-m3/mole)
VP: 3.29E-006 mm Hg (source: MPBPVP)
WS: 3.71E+004 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -1.69 (KowWin est)
Log Kaw used: -13.332 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 11.642
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7421
Biowin2 (Non-Linear Model) : 0.8107
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.9687 (weeks)
Biowin4 (Primary Survey Model) : 3.7716 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.1984
Biowin6 (MITI Non-Linear Model): 0.0663
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5427
Ready Biodegradability Prediction: NO

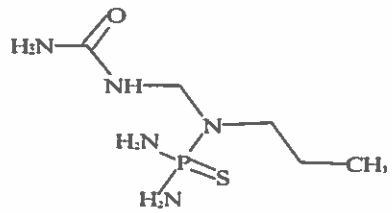
Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  0.00165 Pa (1.24E-005 mm Hg)
 Log Koa (Koawin est  ): 11.642
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.00181
      Octanol/air (Koa) model:  0.108
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.0615
      Mackay model           :  0.127
      Octanol/air (Koa) model:  0.896

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 638.0266 E-12 cm3/molecule-sec
     Half-Life =     0.017 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =    12.070 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.0941 (Junge-Pankow, Mackay avg)
     0.896 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  14.94  L/kg (MCI method)
     Log Koc:  1.174       (MCI method)
     Koc    :  0.6653  L/kg (Kow method)
     Log Koc:  -0.177      (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -3.5501 days (HL = 0.0002818 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.8934)
  Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.8934)
      log Kow used: -1.69 (estimated)

Volatilization from Water:
   Henry LC:  1.14E-015 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 7.944E+011  hours   (3.31E+010 days)
   Half-Life from Model Lake : 8.667E+012  hours   (3.611E+011 days)

Removal In Wastewater Treatment:
   Total removal:                1.85  percent
   Total biodegradation:         0.09  percent
   Total sludge adsorption:      1.75  percent
   Total to Air:                 0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       2.52e-008      0.402        1000
  Water     28.3           360          1000
  Soil      71.6           720          1000
  Sediment  0.0696         3.24e+003    0
    Persistence Time: 659 hr
```

CAS Number:
SMILES : NC(=O)NCN(CCC)P(=S)(N)N
CHEM : K32B
MOL FOR: C5 H16 N5 O1 P1 S1
MOL WT : 225.25

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -2.18

Boiling Pt, Melting Pt, Vapor Pressure Estimations
Boiling Pt (deg C): 379.86 (Adapted Stein &
Melting Pt (deg C): 83.28 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 7.07E-006 (Modified Grain method)
VP (Pa, 25 deg C) : 0.000943 (Modified Grain method)
Subcooled liquid VP: 2.55E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.0034 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 1.161e+005
log Kow used: -2.18 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 8.4272e+005 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Substituted Ureas

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 8.61E-016 atm-m3/mole (8.72E-011 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.805E-011 atm-m3/mole (1.829E-006 Pa-m3/mole)
VP: 7.07E-006 mm Hg (source: MPBPVP)
WS: 1.16E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -2.18 (KowWin est)
Log Kaw used: -13.453 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 11.273
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.6403
Biowin2 (Non-Linear Model) : 0.4527
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.7014 (weeks-months)
Biowin4 (Primary Survey Model) : 3.5228 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.1907
Biowin6 (MITI Non-Linear Model): 0.0648
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.8345
Ready Biodegradability Prediction: NO

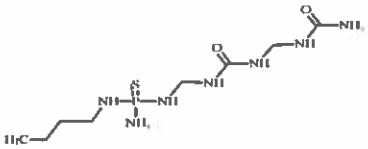
Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  0.0034 Pa (2.55E-005 mm Hg)
 Log Koa (Koawin est  ): 11.273
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.000882
      Octanol/air (Koa) model:  0.046
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.0309
      Mackay model           :  0.0659
      Octanol/air (Koa) model:  0.786

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 458.6136 E-12 cm3/molecule-sec
     Half-Life =     0.023 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =    16.792 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.0484 (Junge-Pankow, Mackay avg)
     0.786 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  10  L/kg (MCI method)
     Log Koc:  1.000       (MCI method)
     Koc    :  0.3564  L/kg (Kow method)
     Log Koc:  -0.448      (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -3.7234 days (HL = 0.0001891 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.8931)
  Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.8931)
      log Kow used: -2.18 (estimated)

Volatilization from Water:
   Henry LC:  8.61E-016 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 1.021E+012  hours   (4.252E+010 days)
   Half-Life from Model Lake : 1.113E+013  hours   (4.639E+011 days)

Removal In Wastewater Treatment:
   Total removal:                1.85  percent
   Total biodegradation:         0.09  percent
   Total sludge adsorption:      1.75  percent
   Total to Air:                 0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       1.06e-008      0.56         1000
  Water     35             900          1000
  Soil      64.9           1.8e+003     1000
  Sediment  0.0835         8.1e+003     0
    Persistence Time: 1.15e+003 hr
```

CAS Number:
SMILES : CCCCNP(=S)(N)NCNC(=O)NCNC(=O)N
CHEM : K32C
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -3.15

Boiling Pt, Melting Pt, Vapor Pressure Estimations
Boiling Pt (deg C): 480.00 (Adapted Stein &
Melting Pt (deg C): 90.27 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 2.06E-008 (Modified Grain method)
VP (Pa, 25 deg C) : 2.74E-006 (Modified Grain method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 2.527e+005
log Kow used: -3.15 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Substituted Ureas

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 5.45E-024 atm-m3/mole (5.52E-019 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 3.340E-014 atm-m3/mole (3.384E-009 Pa-m3/mole)
VP: 2.06E-008 mm Hg (source: MPBPVP)
WS: 2.53E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -3.15 (KowWin est)
Log Kaw used: -21.652 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 18.502
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7078
Biowin2 (Non-Linear Model) : 0.6062
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.8095 (weeks)
Biowin4 (Primary Survey Model) : 3.6676 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.0334
Biowin6 (MITI Non-Linear Model): 0.0134
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5687
Ready Biodegradability Prediction: NO

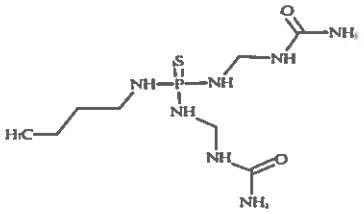
Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  1.17E-005 Pa (8.76E-008 mm Hg)
 Log Koa (Koawin est  ): 18.502
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.257
      Octanol/air (Koa) model:  7.8E+005
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.903
      Mackay model           :  0.954
      Octanol/air (Koa) model:  1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 655.7271 E-12 cm3/molecule-sec
     Half-Life =     0.016 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =    11.744 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.928 (Junge-Pankow, Mackay avg)
     1 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  10  L/kg (MCI method)
     Log Koc:  1.000       (MCI method)
     Koc    :  0.09154  L/kg (Kow method)
     Log Koc:  -1.038      (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -5.4131 days (HL = 3.863e-006 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)
  Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)
      log Kow used: -3.15 (estimated)

Volatilization from Water:
   Henry LC:  5.45E-024 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 1.896E+020  hours   (7.898E+018 days)
   Half-Life from Model Lake : 2.068E+021  hours   (8.616E+019 days)

Removal In Wastewater Treatment:
   Total removal:                1.85  percent
   Total biodegradation:         0.09  percent
   Total sludge adsorption:      1.75  percent
   Total to Air:                 0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       1.26e-015      0.391        1000
  Water     30.6           360          1000
  Soil      69.4           720          1000
  Sediment  0.0688         3.24e+003    0
    Persistence Time: 640 hr
```

CAS Number:
SMILES : CCCCNP(=S)(NCNC(=O)N)NCNC(=O)N
CHEM : K32D
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -3.07

Boiling Pt, Melting Pt, Vapor Pressure Estimation:
Boiling Pt (deg C): 480.00 (Adapted Stein &
Melting Pt (deg C): 90.27 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 2.06E-008 (Modified Grain method)
VP (Pa, 25 deg C) : 2.74E-006 (Modified Grain method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 2.153e+005
log Kow used: -3.07 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Substituted Ureas

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 5.45E-024 atm-m3/mole (5.52E-019 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 3.920E-014 atm-m3/mole (3.972E-009 Pa-m3/mole)
VP: 2.06E-008 mm Hg (source: MPBPVP)
WS: 2.15E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -3.07 (KowWin est)
Log Kaw used: -21.652 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 18.582
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7078
Biowin2 (Non-Linear Model) : 0.6062
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.8095 (weeks)
Biowin4 (Primary Survey Model) : 3.6676 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.0334
Biowin6 (MITI Non-Linear Model): 0.0134
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5687
Ready Biodegradability Prediction: NO

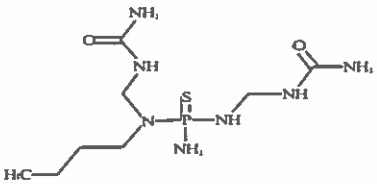
Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  1.17E-005 Pa (8.76E-008 mm Hg)
 Log Koa (Koawin est  ): 18.582
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.257
      Octanol/air (Koa) model:  9.38E+005
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.903
      Mackay model           :  0.954
      Octanol/air (Koa) model:  1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 675.6400 E-12 cm3/molecule-sec
     Half-Life =     0.016 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =    11.398 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.928 (Junge-Pankow, Mackay avg)
     1 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  10.11  L/kg (MCI method)
     Log Koc:  1.005       (MCI method)
     Koc    :  0.1014  L/kg (Kow method)
     Log Koc:  -0.994      (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -5.3881 days (HL = 4.092e-006 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)
  Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)
      log Kow used: -3.07 (estimated)

Volatilization from Water:
   Henry LC:  5.45E-024 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 1.896E+020  hours   (7.898E+018 days)
   Half-Life from Model Lake : 2.068E+021  hours   (8.616E+019 days)

Removal In Wastewater Treatment:
   Total removal:              1.85  percent
   Total biodegradation:       0.09  percent
   Total sludge adsorption:    1.75  percent
   Total to Air:               0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       1.26e-015      0.38          1000
  Water     30.5           360           1000
  Soil      69.4           720           1000
  Sediment  0.0688         3.24e+003     0
    Persistence Time: 641 hr
```

CAS Number:
SMILES : CCCCN(CNC(=O)N)P(=S)(N)NCNC(=O)N
CHEM : K32E
MOL FOR: C8 H22 N7 O2 P1 S1
MOL WT : 311.34

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -3.07

Boiling Pt, Melting Pt, Vapor Pressure Estimations
Boiling Pt (deg C): 480.00 (Adapted Stein &
Melting Pt (deg C): 90.27 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 2.06E-008 (Modified Grain method)
VP (Pa, 25 deg C) : 2.74E-006 (Modified Grain method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-005 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 2.153e+005
log Kow used: -3.07 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Substituted Ureas

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 5.45E-024 atm-m3/mole (5.52E-019 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 3.920E-014 atm-m3/mole (3.972E-009 Pa-m3/mole)
VP: 2.06E-008 mm Hg (source: MPBPVP)
WS: 2.15E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -3.07 (KowWin est)
Log Kaw used: -21.652 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 18.582
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7078
Biowin2 (Non-Linear Model) : 0.6062
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.8095 (weeks)
Biowin4 (Primary Survey Model) : 3.6676 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.0334
Biowin6 (MITI Non-Linear Model): 0.0134
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.5687
Ready Biodegradability Prediction: NO

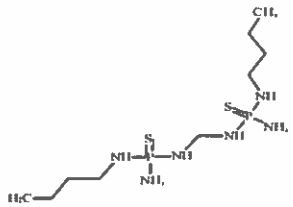
Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  1.17E-005 Pa (8.76E-008 mm Hg)
 Log Koa (Koawin est  ): 18.582
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.257
      Octanol/air (Koa) model:  9.38E+005
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.903
      Mackay model           :  0.954
      Octanol/air (Koa) model:  1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 497.6400 E-12 cm3/molecule-sec
     Half-Life =     0.021 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =    15.475 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.928 (Junge-Pankow, Mackay avg)
     1 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  10  L/kg (MCI method)
     Log Koc:  1.000       (MCI method)
     Koc    :  0.1014  L/kg (Kow method)
     Log Koc:  -0.994      (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -5.3881 days (HL = 4.092e-006 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)
  Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)
      log Kow used: -3.07 (estimated)

Volatilization from Water:
   Henry LC:  5.45E-024 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 1.896E+020  hours   (7.898E+018 days)
   Half-Life from Model Lake : 2.068E+021  hours   (8.616E+019 days)

Removal In Wastewater Treatment:
   Total removal:              1.85  percent
   Total biodegradation:       0.09  percent
   Total sludge adsorption:    1.75  percent
   Total to Air:               0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       1.26e-015      0.516        1000
  Water     30.6           360          1000
  Soil      69.4           720          1000
  Sediment  0.0688         3.24e+003    0
    Persistence Time: 640 hr
```

CAS Number:
SMILES : CCCCNP(=S)(N)NCNP(=S)(N)NCCCC
CHEM : K32F
MOL FOR: C9 H28 N6 P2 S2
MOL WT : 346.43

---------- EPI SUMMARY (v4.11) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------



Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = -0.38

Boiling Pt, Melting Pt, Vapor Pressure Estimations
Boiling Pt (deg C): 448.76 (Adapted Stein &
Melting Pt (deg C): 87.23 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 1.33E-007 (Modified Grain method)
VP (Pa, 25 deg C) : 1.78E-005 (Modified Grain method)
Subcooled liquid VP: 5.28E-007 mm Hg (25 deg C, Mod-Grain method)
: 7.03E-005 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 1.364e+004
log Kow used: -0.38 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 796.03 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 4.74E-016 atm-m3/mole (4.80E-011 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.445E-012 atm-m3/mole (4.504E-007 Pa-m3/mole)
VP: 1.33E-007 mm Hg (source: MPBPVP)
WS: 1.36E+004 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: -0.38 (KowWin est)
Log Kaw used: -13.713 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 13.333
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7995
Biowin2 (Non-Linear Model) : 0.8553
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.0303 (weeks)
Biowin4 (Primary Survey Model) : 3.8861 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.0282
Biowin6 (MITI Non-Linear Model): 0.0118
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.2234
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

```
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  7.04E-005 Pa (5.28E-007 mm Hg)
 Log Koa (Koawin est  ): 13.333
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  0.0426
      Octanol/air (Koa) model:  5.28
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  0.606
      Mackay model           :  0.773
      Octanol/air (Koa) model:  0.998

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant = 1281.6080 E-12 cm3/molecule-sec
     Half-Life =     0.008 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =     6.009 Min
  Ozone Reaction:
     No Ozone Reaction Estimation
  Fraction sorbed to airborne particulates (phi):
     0.69 (Junge-Pankow, Mackay avg)
     0.998 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  107.5  L/kg (MCI method)
     Log Koc:  2.031       (MCI method)
     Koc    :  2.782  L/kg (Kow method)
     Log Koc:  0.444       (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
   Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
  Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -1.8133 days (HL = 0.01537 days)
  Log BCF Arnot-Gobas method (upper trophic) = -0.041 (BCF = 0.9101)
  Log BAF Arnot-Gobas method (upper trophic) = -0.041 (BAF = 0.9101)
      log Kow used: -0.38 (estimated)

Volatilization from Water:
   Henry LC:  4.74E-016 atm-m3/mole  (estimated by Bond SAR Method)
   Half-Life from Model River: 2.299E+012  hours   (9.579E+010 days)
   Half-Life from Model Lake : 2.508E+013  hours   (1.045E+012 days)

Removal In Wastewater Treatment:
   Total removal:              1.85  percent
   Total biodegradation:       0.09  percent
   Total sludge adsorption:    1.76  percent
   Total to Air:               0.00  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)       (hr)        (kg/hr)
  Air       2.28e-008      0.2          1000
  Water     19.2           360          1000
  Soil      80.7           720          1000
  Sediment  0.117          3.24e+003    0
    Persistence Time: 748 hr
```