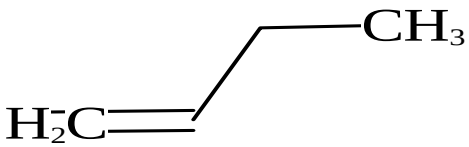
CAS Number: 106-99-0
SMILES : C=CCC
CHEM : Butene
MOL FOR: C4 H8
MOL WT : 56.11

---------- EPI SUMMARY (v4.00) ----------

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 v1.67 estimate) = 2.17
Log Kow (Exper. database match) = 2.40
Exper. Ref: HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 17.57 (Adapted Stein & Brown method)
Melting Pt (deg C): -121.74 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 1.86E+003 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C) : 2.48E+005 (Mean VP of Antoine & Grain methods)
MP (exp database): -145 deg C
BP (exp database): -1.3 deg C
VP (exp database): 2.25E+03 mm Hg (3.00E+005 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):
Water Solubility at 25 deg C (mg/L): 354.8
log Kow used: 2.40 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 221 mg/L (25 deg C)
Exper. Ref: MCAULIFFE,C (1966)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 278 mg/L

ECOSAR Class Program (ECOSAR v1.00):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 2.03E-001 atm-m3/mole (2.06E+004 Pa-m3/mole)
Group Method: 2.68E-001 atm-m3/mole (2.72E+004 Pa-m3/mole)
Exper Database: 2.33E-01 atm-m3/mole (2.36E+004 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.581E-001 atm-m3/mole (1.602E+004 Pa-m3/mole)
VP: 1.86E+003 mm Hg (source: MPBPVP)
WS: 355 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 2.40 (exp database)
Log Kaw used: 0.979 (exp database)
Log Koa (KOAWIN v1.10 estimate): 1.421
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.8293
Biowin2 (Non-Linear Model) : 0.9830
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.3735 (days-weeks)
Biowin4 (Primary Survey Model) : 4.0359 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.6136

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  Biowin6 (MITI Non-Linear Model):   0.8085
Anaerobic Biodegradation Probability:
  Biowin7 (Anaerobic Linear Model):  0.2442
Ready Biodegradability Prediction:   YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
    LOG BioHC Half-Life (days) :   0.4394
    BioHC Half-Life (days)     :   2.7502

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
 Vapor pressure (liquid/subcooled):  3E+005 Pa (2.25E+003 mm Hg)
 Log Koa (Koawin est  ): 1.421
  Kp (particle/gas partition coef. (m3/ug)):
      Mackay model           :  1E-011
      Octanol/air (Koa) model:  6.47E-012
  Fraction sorbed to airborne particulates (phi):
      Junge-Pankow model     :  3.61E-010
      Mackay model           :  8E-010
      Octanol/air (Koa) model:  5.18E-010

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =  27.4013 E-12 cm3/molecule-sec
     Half-Life =     0.586 Days (24-hr day; 0.5E6 OH/cm3)
     Half-Life =    14.052 Hrs
  Ozone Reaction:
     OVERALL Ozone Rate Constant =     1.200000 E-17 cm3/molecule-sec
     Half-Life =     0.955 Days (at 7E11 mol/cm3)
     Half-Life =     22.920 Hrs
  Fraction sorbed to airborne particulates (phi):
     5.81E-010 (Junge-Pankow, Mackay avg)
     5.18E-010 (Koa method)
   Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
     Koc    :  39.6  L/kg (MCI method)
     Log Koc:  1.598      (MCI method)
     Koc    :  120.9  L/kg (Kow method)
     Log Koc:  2.083      (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 v3.00):
  Log BCF from regression-based method = 1.251 (BCF = 17.8 L/kg wet-wt)
  Log Biotransformation Half-life (HL) = -0.3434 days (HL = 0.4536 days)
  Log BCF Arnot-Gobas method (upper trophic) = 1.369 (BCF = 23.39)
  Log BAF Arnot-Gobas method (upper trophic) = 1.369 (BAF = 23.39)
      log Kow used: 2.40 (expkow database)

Volatilization from Water:
   Henry LC:  0.233 atm-m3/mole  (Henry experimental database)
   Half-Life from Model River:     0.7663  hours   (45.98 min)
   Half-Life from Model Lake :      71.17  hours   (2.965 days)

Removal In Wastewater Treatment (recommended maximum 95%):
   Total removal:              98.91  percent
   Total biodegradation:        0.02  percent
   Total sludge adsorption:     0.85  percent
   Total to Air:               98.03  percent
     (using 10000 hr Bio P,A,S)

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)        (hr)       (kg/hr)
  Air       14.3            8.23         1000
  Water     83.6            208          1000
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Soil	1.89	416	1000
Sediment	0.263	1.87e+003	0

Persistence Time: 58.4 hr