

3-vinyltoluene c₉h₁₀ structure



**ASSIGN
BUSTER**

Contents

- Retention Index (Normal Alkane):

Molecular

 C_9H_{10}

Formula

Average mass 118.176 Da

Density

 $0.9 \pm 0.1 \text{ g/cm}^3$

Boiling Point

 $170.0 \pm 10.0 \text{ }^\circ\text{C}$ at
760 mmHg

Flash Point

 $51.1 \pm 0.0 \text{ }^\circ\text{C}$

Molar

 $42.0 \pm 0.3 \text{ cm}^3$

Refractivity

Polarizability

 $16.7 \pm 0.5 \cdot 10^{-24}$
 cm^3

Surface

 $30.7 \pm 3.0 \text{ dyne/cm}$

Tension

Molar Volume $131.7 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

-82-81 °C Alfa Aesar

-86 °C Jean-Claude

Bradley Open Melting

Point Dataset 13501

-86.3 °C Jean-Claude

Bradley Open Melting

Point Dataset 20683

-82 °C Jean-Claude

Bradley Open Melting

Point Dataset 4121

-82-81 °C Alfa

Aesar L08072

- **Experimental Boiling Point:**

170-171 °C Alfa Aesar

170-171 °C Alfa

Aesar L08072

- **Experimental Flash Point:**

51 °CAlfa Aesar

51 °CAlfa Aesar

51 °F (10. 5556 °C)Alfa

AesarL08072

60

°CLabNetworkLN00238

850

- **Experimental Gravity:**

0. 9 g/mLAlfa

AesarL08072

- **Experimental Refraction Index:**

1. 541Alfa

AesarL08072

- Miscellaneous

- **Safety:**

10-36/37/38-65Alfa

AesarL08072

26-37-62Alfa

AesarL08072

3Alfa AesarL08072

DangerAlfa

AesarL08072

DANGER: FLAMMABLE,

irritates skin and

eyesAlfa AesarL08072

H304-H226-H315-

H319-H335Alfa

AesarL08072

HARMFUL /

IRRITANTAlfa

AesarL08072

P210-P301+P310-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

AesarL08072

- Gas Chromatography

- **Retention Index (Kovats):**

996 (estimated with

error: 55)NIST

Spectramainlib_2023,

replib_118474,

replib_231965

956 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column type: Capillary;

Start T: 0 C; CAS no:

100801; Active phase:

OV-101; Data type:

Kovats RI; Authors:

Skrbic, B. D.; Vojinovic-

Miloradov, M. B., A

contribution to the

qualitative GC analysis

of some non-

chlorinated xenobiotic

chemicals in waste

waters, Water Sci.

Technol., 30(3), 1994,

91-93.)NIST Spectranist

ri

977 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 100 m;
Column type: Capillary;
Start T: 96 C; CAS no:
100801; Active phase:
Squalane; Carrier gas:
He; Data type: Kovats
RI; Authors:
Kugucheva, E. E.;
Mashinsky, V. I.,
Retention Indices of
Aromatic Hydrocarbons
on Capillary Columns
with Squalan and
Polyphenyl Ether, Zh.
Anal. Khim. (Rus),
38(11), 1983, 2023-
2026., Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0.25
mm; Column length: 15

m; Column type:
Capillary; Start T: 70 C;
CAS no: 100801; Active
phase: SE-30; Carrier
gas: N2; Data type:
Kovats RI; Authors:
Toth, T., Use of
capillary gas
chromatography in
collecting retention and
chemical information
for the analysis of
complex petrochemical
mixtures, J.
Chromatogr., 279,
1983, 157-165.)NIST
Spectranist ri

960. 5 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0. 25
mm; Column length: 15
m; Column type:
Capillary; Start T: 70 C;

CAS no: 100801; Active

phase: SE-30; Carrier

gas: N2; Data type:

Kovats RI; Authors:

Toth, T., Use of

capillary gas

chromatography in

collecting retention and

chemical information

for the analysis of

complex petrochemical

mixtures, J.

Chromatogr., 279,

1983, 157-165.)NIST

Spectranist ri

1000 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0.5

mm; Column length:

100 m; Column type:

Capillary; Start T: 130

C; CAS no: 100801;

Active phase: SE-30;

Data type: Kovats RI;
Authors: Bredael, P.,
Retention indices of
hydrocarbons on SE-30,
J. Hi. Res. Chromatogr.
& Chromatogr. Comm.,
5, 1982, 325-328.)NIST
Spectranist ri

982 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0.5
mm; Column length:
100 m; Column type:
Capillary; Start T: 80 C;
CAS no: 100801; Active
phase: SE-30; Data
type: Kovats RI;
Authors: Bredael, P.,
Retention indices of
hydrocarbons on SE-30,
J. Hi. Res. Chromatogr.
& Chromatogr. Comm.,
5, 1982, 325-328.)NIST

Spectranist ri

985. 9 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0. 3

mm; Column length: 50

m; Column type:

Capillary; Start T: 100

C; CAS no: 100801;

Active phase: OV-101;

Carrier gas: N2; Data

type: Kovats RI;

Authors: Gerasimenko,

V. A.; Kirilenko, A. V.;

Nabivach, V. M.,

Capillary gas

chromatography of

aromatic compounds

found in coal tar

fractions, J.

Chromatogr., 208,

1981, 9-16.)NIST

Spectranist ri

991. 4 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0. 3
mm; Column length: 50
m; Column type:
Capillary; Start T: 120
C; CAS no: 100801;
Active phase: OV-101;
Carrier gas: N2; Data
type: Kovats RI;
Authors: Gerasimenko,
V. A.; Kirilenko, A. V.;
Nabivach, V. M.,
Capillary gas
chromatography of
aromatic compounds
found in coal tar
fractions, J.
Chromatogr., 208,
1981, 9-16.)NIST
Spectranist ri

997. 8 (Program type:
Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0.3

mm; Column length: 50

m; Column type:

Capillary; Start T: 140

C; CAS no: 100801;

Active phase: OV-101;

Carrier gas: N2; Data

type: Kovats RI;

Authors: Gerasimenko,

V. A.; Kirilenko, A. V.;

Nabivach, V. M.,

Capillary gas

chromatography of

aromatic compounds

found in coal tar

fractions, J.

Chromatogr., 208,

1981, 9-16.)NIST

Spectranist ri

972. 7 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0.5
mm; Column length:
25.5 m; Column type:
Capillary; Start T: 65 C;
CAS no: 100801; Active
phase: SE-30; Carrier
gas: He; Data type:
Kovats RI; Authors:
Svob, V.; Deur-Siftar,
D.; Cramers, C. A.,
Mechanisms of the
thermal degradation of
alkylbenzenes, J.
Chromatogr., 91, 1974,
659-675.)NIST
Spectranist ri

973.2 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0.5
mm; Column length:
25.5 m; Column type:
Capillary; Start T: 65 C;
CAS no: 100801; Active

phase: SE-30; Carrier
gas: He; Data type:
Kovats RI; Authors:
Svob, V.; Deur-Siftar,
D., Kovats Retention
Indices in the
Identification of
Alkylbenzene
Degradation Products,
J. Chromatogr., 91,
1974, 677-689.,
Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0.5
mm; Column length:
25.5 m; Column type:
Capillary; Start T: 65 C;
CAS no: 100801; Active
phase: SE-30; Carrier
gas: He; Data type:
Kovats RI; Authors:
Svob, V.; Deur-Siftar,
D.; Cramers, C. A.,
Mechanisms of the

thermal degradation of
alkylbenzenes, J.

Chromatogr., 91, 1974,

659-675.)NIST

Spectranist ri

980 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 100 m;

Column type: Capillary;

Start T: 106 C; CAS no:

100801; Active phase:

Squalane; Carrier gas:

He; Data type: Kovats

RI; Authors:

Kugucheva, E. E.;

Mashinsky, V. I.,

Retention Indices of

Aromatic Hydrocarbons

on Capillary Columns

with Squalan and

Polyphenyl Ether, Zh.

Anal. Khim. (Rus),

38(11), 1983, 2023-

2026.)NIST Spectranist

ri

976. 3 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0. 25

mm; Column length: 50

m; Column type:

Capillary; Start T: 86 C;

CAS no: 100801; Active

phase: Squalane;

Carrier gas: N2; Data

type: Kovats RI;

Authors: Macak, J.;

Nabivach, V.; Buryan,

P.; Sindler, S.,

Dependence of

retention indices of

alkylbenzenes on their

molecular structure, J.

Chromatogr., 234,

1982, 285-302.,

Program type:

Isothermal; Col... (show

more)umn class: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 50
m; Column type:
Capillary; Start T: 86 C;
CAS no: 100801; Active
phase: Squalane; Data
type: Kovats RI;
Authors: Nabivach, V.
M.; Bur'yan, P.; Matsak,
I., Retention indices of
aromatic hydrocarbons
on a squalane capillary
column, Zh. Anal.
Khim., 33(7), 1978,
1108-1113, In original
1416-1422.)NIST
Spectranist ri

978.7 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 50

m; Column type:
Capillary; Start T: 96 C;
CAS no: 100801; Active
phase: Squalane;
Carrier gas: N2; Data
type: Kovats RI;
Authors: Macak, J.;
Nabivach, V.; Buryan,
P.; Sindler, S.,
Dependence of
retention indices of
alkylbenzenes on their
molecular structure, J.
Chromatogr., 234,
1982, 285-302.,
Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 50
m; Column type:
Capillary; Start T: 96 C;
CAS no: 100801; Active
phase: Squalane; Data
type: Kovats RI;

Authors: Nabivach, V.
M.; Bur'yan, P.; Matsak,
I., Retention indices of
aromatic hydrocarbons
on a squalane capillary
column, Zh. Anal.
Khim., 33(7), 1978,
1108-1113, In original
1416-1422.)NIST
Spectranist ri

1385. 2 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
diameter: 0. 32 mm;
Column length: 50 m;
Column type: Capillary;
Start T: 110 C; CAS no:
100801; Active phase:
Carbowax 20M; Carrier
gas: N2; Phase
thickness: 0. 3 um;
Data type: Kovats RI;
Authors: Boneva, S.;
Vassilev, K., Gas

chromatographic
separation of
epoxystyrenes on
carbowax 20 M
capillary column,
Chromatographia,
43(3/4), 1996, 208-
210.)NIST Spectranist ri
1396. 8 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
diameter: 0. 32 mm;
Column length: 50 m;
Column type: Capillary;
Start T: 120 C; CAS no:
100801; Active phase:
Carbowax 20M; Carrier
gas: N2; Phase
thickness: 0. 3 um;
Data type: Kovats RI;
Authors: Boneva, S.;
Vassilev, K., Gas
chromatographic
separation of

epoxystyrenes on
carbowax 20 M
capillary column,
Chromatographia,
43(3/4), 1996, 208-
210.)NIST Spectranist ri

1348. 1 (Program type:
Isothermal; Col... (show
more)umn class:

Standard polar; Column
diameter: 0. 3 mm;

Column length: 30 m;

Column type: Capillary;

Start T: 70 C; CAS no:

100801; Active phase:

PEG-20M; Carrier gas:

N2; Data type: Kovats

RI; Authors: Toth, T.,

Use of capillary gas

chromatography in

collecting retention and

chemical information

for the analysis of

complex petrochemical

mixtures, J.

Chromatogr., 279,
1983, 157-165.)NIST
Spectranist ri

1388. 1 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
type: Packed; Start T:
150 C; CAS no:
100801; Active phase:
Carbowax 20M;
Substrate: Chromosorb
W, AW-DMCS; Data
type: Kovats RI;
Authors: Ellis, T. S.;
Still, R. H., Thermal
degradation of
polymers. XXI. Vacuum
pyrolysis of poly(m-N,
N-
dimethylaminostyrene)
; the products volatile
at pyrolysis
temperature, liquid at
room temperature, J.

Appl. Polym. Sci., 23,
1979, 2837-2854.)NIST

Spectranist ri

1387. 4 (Program type:
Isothermal; Col... (show
more)umn class:

Standard polar; Column
type: Packed; Start T:

150 C; CAS no:

100801; Active phase:

Carbowax 20M;

Substrate: Chromosorb

W, AW-DMCS; Data

type: Kovats RI;

Authors: Ellis, T. S.;

Still, R. H., Thermal

degradation of

polymers. XXI. Vacuum

pyrolysis of poly(m-N,

N-

dimethylaminostyrene)

; the products volatile

at pyrolysis

temperature, liquid at

room temperature, J.

Appl. Polym. Sci., 23,
1979, 2837-2854.)NIST
Spectranist ri

- **Retention Index (Lee):**

156. 2 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 60
m; Column type:
Capillary; CAS no:
100801; Active phase:
DB-5MS; Data type:
Lee RI; Authors: Aracil,
I.; Font, R.; Conesa, J.
A., Semivolatile and
volatile compounds
from the pyrolysis and
combustion of polyvinyl
chloride, J. Anal. Appl.
Pyrolysis, 74, 2005,
465-478.)NIST
Spectranist ri

158. 1 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 2
mm; Column length: 50
m; Column type:
Capillary; Heat rate: 5
K/min; Start T: 50 C;
End T: 280 C; End time:
30 min; CAS no:
100801; Active phase:
HP-5MS; Carrier gas:
He; Phase thickness: 0.
33 um; Data type: Lee
RI; Authors: Wang, S.-
F.; Liu, B.-Z.; Sun, K.-J.;
Su, Q.-D., Gas
chromatographic-mass
spectrometric
determination of
polycyclic aromatic
hydrocarbons formed
during the pyrolysis of
phenylalanine, J.
Chromatogr. A, 1025,

2004, 255-261.)NIST

Spectranist ri

- **Retention Index (Normal Alkane):**

960 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Capillary;

CAS no: 100801; Active

phase:

Polymethylsiloxane,

(PMS-20000); Data

type: Normal alkane RI;

Authors: Cornwell, E.;

Cordano, G., Nueva

proposicion para

predecir datos de

retencion obtenidos

mediante

cromatografia de gases

de hidrocarburos

derivados de las

naftas, Revista de la

Sociedad Quimica de

Mexico, 47(1), 2003,

38-43.)NIST Spectranist

ri

977 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Capillary;

CAS no: 100801; Active

phase:

Polymethylsiloxane,

(PMS-20000); Data

type: Normal alkane RI;

Authors: Cornwell, E.;

Cordano, G., Nueva

proposicion para

predecir datos de

retencion obtenidos

mediante

cromatografia de gases

de hidrocarburos

derivados de las

naftas, Revista de la

Sociedad Quimica de

Mexico, 47(1), 2003,

38-43.)NIST Spectranist

ri

981 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 50 C; End T:

160 C; CAS no:

100801; Active phase:

OV-1; Data type:

Normal alkane RI;

Authors: Orav, A.;

Kailas, T.; Muurisepp,

M.; Kann, J.,

Composition of the oil

from waste tires. 2.

Fraction boiling at 160-

180 0C, Proc. Estonian

Acad. Sci. Chem.,

48(3), 1999, 136-

140.)NIST Spectranist ri

976 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0.20

mm; Column length: 50

m; Column type:

Capillary; Heat rate: 1

K/min; Start T: 30 C;

End T: 100 C; Start

time: 6 min; CAS no:

100801; Active phase:

OV-101; Carrier gas:

Helium; Phase

thickness: 0.50 um;

Data type: Normal

alkane RI; Authors:

Orav, A.; Kailas, T.;

Muurisepp, M.; Kann, J.,

Composition of the oil

from waste tires. 1.

Fraction boiling at y_p to

160 °C, Proc. Estonian

Acad. Sci. Chem.,

48(1), 1999, 30-

39.)NIST Spectranist ri

991 (Program type:

Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.2
mm; Column length: 50
m; Column type:
Capillary; Heat rate: 5
K/min; Start T: 50 C;
End T: 280 C; End time:
30 min; CAS no:
100801; Active phase:
HP-5MS; Carrier gas:
He; Phase thickness: 0.
33 um; Data type:
Normal alkane RI;
Authors: Wang, S.-F.;
Liu, B.-Z.; Sun, K.-J.; Su,
Q.-D., Gas
chromatographic-mass
spectrometric
determination of
polycyclic aromatic
hydrocarbons formed
during the pyrolysis of
phenylalanine, J.
Chromatogr. A, 1025,

2004, 255-261.)NIST

Spectranist ri

1348 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

type: Capillary; CAS no:

100801; Active phase:

Carbowax 20M; Data

type: Normal alkane RI;

Authors: Cornwell, E.;

Cordano, G., Nueva

proposicion para

predecir datos de

retencion obtenidos

mediante

cromatografia de gases

de hidrocarburos

derivados de las

naftas, Revista de la

Sociedad Quimica de

Mexico, 47(1), 2003,

38-43.)NIST Spectranist

ri

Predicted data is generated using the ACD/Labs Percepta Platform -
PhysChem Module

Density:	0. 9±0. 1 g/cm ³
Boiling Point:	170. 0±10. 0 °C at 760 mmHg
Vapour Pressure:	2. 0±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	39. 0±0. 8 kJ/mol
Flash Point:	51. 1±0. 0 °C
Index of Refraction:	1. 551
Molar Refractivity:	42. 0±0. 3 cm ³
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0
ACD/LogP:	3. 16
ACD/LogD (pH 5. 5):	3. 46
ACD/BCF (pH 5. 5):	251. 43

ACD/KOC (pH 5. 5):	1818. 99
ACD/LogD (pH 7. 4):	3. 46
ACD/BCF (pH 7. 4):	251. 43
ACD/KOC (pH 7. 4):	1818. 99
Polar Surface Area:	0 Å ²
Polarizability:	16. 7±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	30. 7±3. 0 dyne/cm
Molar Volume:	131. 7±3. 0 cm ³

Predicted data is generated using the US Environmental Protection Agency's
EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 3. 44Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 168. 39 (Adapted Stein & Brown method)Melting Pt (deg C): -30. 07 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 08 (Mean VP of Antoine & Grain methods)MP (exp database): -86. 3 deg CBP (exp database): 164 deg CVP (exp database): 1. 70E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 117. 1log Kow used: 3. 44 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 89 mg/L (25 deg C)Exper. Ref: YAWS, CL ET AL (1990)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 54. 156 mg/LWat Sol (Exper. database match) = 89. 00Exper. Ref: YAWS, CL ET AL (1990)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 05E-003 atm-m3/moleGroup Method: 3. 01E-003 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 762E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 44 (KowWin est)Log Kaw used: -0. 904 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 344Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7460Biowin2 (Non-Linear Model) : 0. 8708Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8632 (weeks)Biowin4 (Primary Survey Model) : 3. 6087 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4535Biowin6 (MITI Non-Linear Model): 0. 4968Anaerobic Biodegradation Probability: Biowin7

<https://assignbuster.com/3-vinyltoluene-c9h10-structure/>

(Anaerobic Linear Model): -0.1380 Ready Biodegradability Prediction:
NO Hydrocarbon Biodegradation (BioHCwin v1.01): LOG BioHC Half-Life (days) :
0.5907 BioHC Half-Life (days) : 3.8971 Sorption to aerosols (25 Dec C)
[AEROWIN v1.00]: Vapor pressure (liquid/subcooled): 227 Pa (1.7 mm Hg) Log
Koa (Koawin est) : 4.344 Kp (particle/gas partition coef. (m³/ug)): Mackay
model : 1.32E-008 Octanol/air (Koa) model: 5.42E-009 Fraction sorbed to
airborne particulates (phi): Junge-Pankow model : 4.78E-007 Mackay model :
1.06E-006 Octanol/air (Koa) model: 4.34E-007 Atmospheric Oxidation (25 deg
C) [AopWin v1.92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant =
31.2216 E-12 cm³/mole-sec Half-Life = 0.343 Days (12-hr day; 1.5E6
OH/cm³) Half-Life = 4.111 Hrs Ozone Reaction: OVERALL Ozone Rate Constant = 2.
100000 E-17 cm³/mole-sec Half-Life = 0.546 Days (at 7E11 mol/cm³) Half-
Life = 13.097 Hrs Fraction sorbed to airborne particulates (phi): 7.68E-007
(Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric
oxidation Soil Adsorption Coefficient (PCKOCWIN v1.66): Koc : 838.6 Log Koc:
2.924 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
Rate constants can NOT be estimated for this structure! Bioaccumulation
Estimates from Log Kow (BCFWIN v2.17): Log BCF from regression-based method
= 1.951 (BCF = 89.24) log Kow used: 3.44 (estimated) Volatilization from
Water: Henry LC: 0.00301 atm-m³/mole (estimated by Group SAR Method) Half-
Life from Model River: 1.321 hours Half-Life from Model Lake : 105.6 hours
(4.398 days) Removal In Wastewater Treatment: Total removal: 58.19
percent Total biodegradation: 0.10 percent Total sludge adsorption: 8.66
percent Total to Air: 49.43 percent (using 10000 hr Bio P, A, S) Level III
Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 1.
31 5.05 1000 Water 21 360 1000 Soil 76.9 720 1000 Sediment 0.824 3.
24e+003 0 Persistence Time: 305 hr

[Click to predict properties on the Chemicalize site](https://assignbuster.com/3-vinyltoluene-c9h10-structure/)