

2,4,6-trichloroanisole  
c7h5cl3o structure



**ASSIGN  
BUSTER**

## Contents

- Retention Index (Linear):

Molecular  
Formula             $C_7H_5Cl_3O$

Average mass 211. 473 Da

Density             $1.4 \pm 0.1 \text{ g/cm}^3$

Boiling Point      $246.0 \pm 0.0 \text{ }^\circ\text{C}$  at  
760 mmHg

Flash Point        $100.4 \pm 26.0 \text{ }^\circ\text{C}$

Molar  
Refractivity        $47.6 \pm 0.3 \text{ cm}^3$

Polarizability     $18.9 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface  
Tension             $38.4 \pm 3.0 \text{ dyne/cm}$

Molar Volume     $149.3 \pm 3.0 \text{ cm}^3$

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

- Predicted - ChemAxon
- Predicted - Mcule
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

60 °CIT0867

60-62 °COxford

University Chemical

Safety Data (No longer  
updated)More details

61 °CJean-Claude

Bradley Open Melting

Point Dataset14933

61.5 °CJean-Claude

Bradley Open Melting

Point Dataset21028

61-62

°CFooDBFDB000814

- **Experimental Boiling Point:**

132 °COxford

University Chemical

Safety Data (No longer

updated)More details

738 °C / 240 mmHg

(840. 0944 °C / 760

mmHg)FooDBFDB0008

14

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

- 60 °CTCI

- 60

- °CTCIT0867

- Miscellaneous

- **Appearance:**

- white or off-white

- fibrous powderOxford

- University Chemical

- Safety Data (No longer

- updated)More details

- **Stability:**

- Stable. Incompatible

- with strong oxidizing

- agents. Oxford

- University Chemical

Safety Data (No longer  
updated)More details

- **Safety:**

Safety glasses,  
adequate ventilation.

Oxford University

Chemical Safety Data

(No longer  
updated)More details

- Gas Chromatography

- **Retention Index (Kovats):**

1409 (estimated with  
error: 89)NIST

Spectramainlib\_333450

, replib\_69785,

replib\_100136,

replib\_238004,

replib\_249011

1339 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0. 25

mm; Column type:  
Capillary; CAS no:  
87401; Active phase:  
Methyl Silicone; Data  
type: Kovats RI;  
Authors: Staples, E. J.,  
Ultrahigh-speed  
chromatography and  
virtual chemical  
sensors for detecting  
explosives and  
chemical warfare  
agents, IEEE Sens. J.,  
5(4), 2005, 622-  
631.)NIST Spectranist ri  
1319 (Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;  
Column diameter: 0.3  
mm; Column length: 25  
m; Column type:  
Capillary; Start T: 140  
C; CAS no: 87401;  
Active phase: SE-30;

Carrier gas: N2; Data  
type: Kovats RI;  
Authors: Korhonen, I. O.  
O., Gas-Liquid  
Chromatographic  
Analyses. XXVIII.  
Capillary Column  
Studies of Chlorinated  
Anisoles, J.  
Chromatogr., 294,  
1984, 99-116.)NIST  
Spectranist ri  
  
1333 (Program type:  
Isothermal; Col... (show  
more)umn class:  
Standard non-polar;  
Column diameter: 0.3  
mm; Column length: 25  
m; Column type:  
Capillary; Start T: 160  
C; CAS no: 87401;  
Active phase: SE-30;  
Carrier gas: N2; Data  
type: Kovats RI;  
Authors: Korhonen, I. O.

O., Gas-Liquid

Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

1350 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0.3

mm; Column length: 25

m; Column type:

Capillary; Start T: 180

C; CAS no: 87401;

Active phase: SE-30;

Carrier gas: N<sub>2</sub>; Data

type: Kovats RI;

Authors: Korhonen, I. O.

O., Gas-Liquid

Chromatographic

Analyses. XXVIII.



Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

1813 (Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

diameter: 0. 32 mm;

Column length: 25 m;

Column type: Capillary;

Start T: 140 C; CAS no:

87401; Active phase:

OV-351; Carrier gas:

N2; Data type: Kovats

RI; Authors: Korhonen,

I. O. O., Gas-Liquid

Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

1837 (Program type:

Isothermal; Col... (show  
more)umn class:

Standard polar; Column  
diameter: 0. 32 mm;

Column length: 25 m;

Column type: Capillary;

Start T: 160 C; CAS no:

87401; Active phase:

OV-351; Carrier gas:

N2; Data type: Kovats

RI; Authors: Korhonen,

I. O. O., Gas-Liquid

Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

1842 (Program type:

Isothermal; Col... (show  
more)umn class:

Standard polar; Column  
diameter: 0. 32 mm;

Column length: 25 m;

Column type: Capillary;

Start T: 180 C; CAS no:

87401; Active phase:

OV-351; Carrier gas:

N2; Data type: Kovats

RI; Authors: Korhonen,

I. O. O., Gas-Liquid

Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

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

1322 (Program type:

Complex; Column...

(show more)class:

Standard non-polar;

Column diameter: 0.25  
mm; Column length: 55  
m; Column type:  
Capillary; Description:  
40C(3min) => 20C/min  
=> 80C => 2C/min=>  
240C(45min); CAS no:  
87401; Active phase:  
CP Sil 2; Carrier gas:  
N2; Phase thickness: 0.  
25 um; Data type:  
Normal alkane RI;  
Authors: Fuhrer, U.;  
Deissler, A.;  
Schreitmuller, J.;  
Ballschmiter, K.,  
Analysis of Halogenated  
Methoxybenzenes and  
Hexachlorobenzene  
(HCB) in the Picogram  
m-3 Range in Marine  
Air, Chromatographia,  
45, 1997, 414-  
427.)NIST Spectranist ri  
1298 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0. 32

mm; Column length: 25

m; Column type:

Capillary; Heat rate: 3

K/min; Start T: 80 C;

End T: 260 C; CAS no:

87401; Active phase:

Ultra-1; Carrier gas: He;

Phase thickness: 0. 25

um; Data type: Normal

alkane RI; Authors:

Okumura, T., retention

indices of

environmental

chemicals on methyl

silicone capillary

column, Journal of

Environmental

Chemistry (Japan), 1(2),

1991, 333-358.)NIST

Spectranist ri

1307. 9 (Program type:

Isothermal; Col... (show  
more)umn class:

Standard non-polar;

Column length: 1. 8 m;

Column type: Packed;

CAS no: 87401; Active

phase: OV-101; Carrier

gas: N2; Substrate:

Chromosorb W HP; Data

type: Normal alkane RI;

Authors: Yurawecz, M.

P.; Puma, B. J., Gas

chromatographic

determination of

electron capture

sensitive volatile

industrial chemical

residues in foods, using

AOAC pesticide

multiresidue extraction

and cleanup

procedures, J. Ass.

Offic. Anal. Chem,

69(1), 1986, 80-

86.)NIST Spectranist ri

1330 (Program type:  
Complex; Column...  
(show more)class:  
Semi-standard non-  
polar; Column  
diameter: 0.32 mm;  
Column length: 30 m;  
Column type: Capillary;  
Description: 40 0C ^ 2  
0C/min -> 12 0C/min ->  
105 0C ^ 6 0C/min ->  
220 0C (20 min); CAS  
no: 87401; Active  
phase: DB-5; Carrier  
gas: Hydrogen; Phase  
thickness: 0.50 um;  
Data type: Normal  
alkane RI; Authors:  
Prat, C.; Trias, R.;  
Cullere, L.; Escudero,  
A.; Antico, E.; BAneras,  
L., Off-odor compounds  
produced in cork by  
isolated bacteria and  
fungi: a gas  
chromatography - mass

spectrometry and gas  
chromatography -  
olfactometry study, J.  
Agric. Food Chem.,  
57(16), 2009, 7473-  
7479.)NIST Spectranist  
ri

1291 (Program type:  
Ramp; Column cl...  
(show more)ass: Semi-  
standard non-polar;  
Column diameter: 0.3  
mm; Column length: 30  
m; Column type:  
Capillary; Heat rate: 16  
K/min; Start T: 80 C;  
End T: 250 C; CAS no:  
87401; Active phase:  
DB-5; Carrier gas: H2;  
Data type: Normal  
alkane RI; Authors:  
Spadone, J.-C.;  
Takeoka, G.; Liardon,  
R., Analytical  
Investigation of Rio Off-



Flavor in Green Coffee,  
J. Agric. Food Chem.,  
38(1), 1990, 226-  
233.)NIST Spectranist ri  
1345 (Program type:  
Ramp; Column cl...  
(show more)ass: Semi-  
standard non-polar;  
Column diameter: 0.3  
mm; Column length: 50  
m; Column type:  
Capillary; Heat rate: 16  
K/min; Start T: 80 C;  
End T: 250 C; CAS no:  
87401; Active phase:  
HP-5; Carrier gas: H2;  
Data type: Normal  
alkane RI; Authors:  
Spadone, J.-C.;  
Takeoka, G.; Liardon,  
R., Analytical  
Investigation of Rio Off-  
Flavor in Green Coffee,  
J. Agric. Food Chem.,  
38(1), 1990, 226-

233.)NIST Spectranist ri

1806 (Program type:

Complex; Column...

(show more)class:

Standard polar; Column

diameter: 0. 32 mm;

Column length: 30 m;

Column type: Capillary;

Description: 40 0C (5

min) ^ 4 0C/min -> 100

0C ^ 6 0C/min -> 220

0C (40 min); CAS no:

87401; Active phase:

DB-Wax; Phase

thickness: 0. 50 um;

Data type: Normal

alkane RI; Authors:

Ferreira, V.; Juan, F. S.;

Escudero, A.; Cullere,

L.; Fernandez-Zurbano,

P.; Saenz-Navajas, M.

P.; Cacho, J., Modeling

quality of premium

Spanish red wines from

gas chromatography-

olfactometry data, J.  
Agr. Food. Chem.,  
57(16), 2009, 7490-  
7498.)NIST Spectranist  
ri

1832 (Program type:  
Complex; Column...  
(show more)class:  
Standard polar; Column  
diameter: 0.32 mm;  
Column length: 30 m;  
Column type: Capillary;  
Description: 40 0C ^ 2  
0C/min -> 12 0C/min ->  
105 0C ^ 6 0C/min ->  
220 0C (20 min); CAS  
no: 87401; Active  
phase: DB-Wax; Carrier  
gas: Hydrogen; Phase  
thickness: 0.50 um;  
Data type: Normal  
alkane RI; Authors:  
Prat, C.; Trias, R.;  
Cullere, L.; Escudero,  
A.; Antico, E.; BAneras,

L., Off-odor compounds  
produced in cork by  
isolated bacteria and  
fungi: a gas  
chromatography - mass  
spectrometry and gas  
chromatography -  
olfactometry study, J.  
Agric. Food Chem.,  
57(16), 2009, 7473-  
7479.)NIST Spectranist  
ri

1812 (Program type:  
Complex; Column...  
(show more)class:  
Standard polar; Column  
diameter: 0.25 mm;  
Column length: 30 m;  
Column type: Capillary;  
Description: 25C(8min)  
=> 4C/min => 60C =>  
6C/min => 160C =>  
20C/min => 200C; CAS  
no: 87401; Active  
phase: DB-Wax; Carrier

gas: He; Phase

thickness: 0.25 um;

Data type: Normal

alkane RI; Authors:

Caldentey, P.; Daria

Fumi, M.; Mazzoleni, V.;

Careri, M., Volatile

compounds produced

by microorganisms

isolated from cork,

Flavour Fragr. J., 13,

1998, 185-188.)NIST

Spectranist ri

- **Retention Index (Linear):**

1331 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Capillary;

CAS no: 87401; Active

phase: PONA; Data

type: Linear RI;

Authors: Cantergiani,

E.; Brevard, H.; Krebs,

Y.; Feria-Morales, A.;

Amado, R.; Yeretian,  
C., Characterisation of  
the aroma of green  
Mexican coffee and  
identification of  
mouldy/earthy defect,  
Eur. Food Res. Technol.,  
212, 2001, 648-  
657.)NIST Spectranist ri

1305 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0.3  
mm; Column length: 25  
m; Column type:  
Capillary; Heat rate: 2  
K/min; Start T: 100 C;  
CAS no: 87401; Active  
phase: SE-30; Carrier  
gas: N2; Data type:  
Linear RI; Authors:  
Korhonen, I. O. O., Gas-  
Liquid Chromatographic  
Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

1319 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0.3

mm; Column length: 25

m; Column type:

Capillary; Heat rate: 6

K/min; Start T: 100 C;

CAS no: 87401; Active

phase: SE-30; Carrier

gas: N2; Data type:

Linear RI; Authors:

Korhonen, I. O. O., Gas-

Liquid Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,  
1984, 99-116.)NIST  
Spectranist ri  
  
1327 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard non-polar;  
Column diameter: 0.3  
mm; Column length: 25  
m; Column type:  
Capillary; Heat rate: 10  
K/min; Start T: 100 C;  
CAS no: 87401; Active  
phase: SE-30; Carrier  
gas: N2; Data type:  
Linear RI; Authors:  
Korhonen, I. O. O., Gas-  
Liquid Chromatographic  
Analyses. XXVIII.  
Capillary Column  
Studies of Chlorinated  
Anisoles, J.  
Chromatogr., 294,  
1984, 99-116.)NIST  
Spectranist ri



1350. 8 (Program type:

Complex; Column...

(show more)class:

Semi-standard non-

polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

Description: Multi-step

temperature program;

T(initial)= 60C;

T(final)= 270C; CAS no:

87401; Active phase:

VF-5MS; Carrier gas:

He; Phase thickness: 0.

25 um; Data type:

Linear RI; Authors:

Tret'yakov, K. V.,

Retention Data. NIST

Mass Spectrometry

Data Center.,

2007.)NIST Spectranist

ri

1817 (Program type:

Complex; Column...

(show more)class:

Standard polar; Column

diameter: 0.25 mm;

Column length: 30 m;

Column type: Capillary;

Description: 20C(30s)

=; fast=; 60C =;

4C/min =; 220C

(20min); CAS no:

87401; Active phase:

DB-Wax; Phase

thickness: 0.25 µm;

Data type: Linear RI;

Authors: Cantergiani,

E.; Brevard, H.; Krebs,

Y.; Feria-Morales, A.;

Amado, R.; Yeretzian,

C., Characterisation of

the aroma of green

Mexican coffee and

identification of

mouldy/earthy defect,

Eur. Food Res. Technol.,

212, 2001, 648-

657.)NIST Spectranist ri

1775 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard polar; Column  
diameter: 0.32 mm;  
Column length: 25 m;  
Column type: Capillary;  
Heat rate: 2 K/min;  
Start T: 100 C; CAS no:  
87401; Active phase:  
OV-351; Carrier gas:  
N2; Data type: Linear  
RI; Authors: Korhonen,  
I. O. O., Gas-Liquid  
Chromatographic  
Analyses. XXVIII.  
Capillary Column  
Studies of Chlorinated  
Anisoles, J.  
Chromatogr., 294,  
1984, 99-116.)NIST  
Spectranist ri

1794 (Program type:  
Ramp; Column cl...  
(show more)ass:

Standard polar; Column  
diameter: 0.32 mm;  
Column length: 25 m;  
Column type: Capillary;  
Heat rate: 6 K/min;  
Start T: 100 C; CAS no:  
87401; Active phase:  
OV-351; Carrier gas:  
N2; Data type: Linear  
RI; Authors: Korhonen,  
I. O. O., Gas-Liquid  
Chromatographic  
Analyses. XXVIII.  
Capillary Column  
Studies of Chlorinated  
Anisoles, J.  
Chromatogr., 294,  
1984, 99-116.)NIST  
Spectranist ri  
  
1805 (Program type:  
Ramp; Column cl...  
(show more)ass:  
Standard polar; Column  
diameter: 0.32 mm;  
Column length: 25 m;

Column type: Capillary;

Heat rate: 10 K/min;

Start T: 100 C; CAS no:

87401; Active phase:

OV-351; Carrier gas:

N2; Data type: Linear

RI; Authors: Korhonen,

I. O. O., Gas-Liquid

Chromatographic

Analyses. XXVIII.

Capillary Column

Studies of Chlorinated

Anisoles, J.

Chromatogr., 294,

1984, 99-116.)NIST

Spectranist ri

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

Density:	1. 4±0. 1 g/cm <sup>3</sup>
Boiling Point:	246. 0±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 4 mmHg at 25°C
Enthalpy of Vaporization:	46. 4±3. 0 kJ/mol

Flash Point:	100. 4±26. 0 °C
Index of Refraction:	1. 551
Molar Refractivity:	47. 6±0. 3 cm <sup>3</sup>
#H bond acceptors:	1
#H bond donors:	0
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0
ACD/LogP:	3. 95
ACD/LogD (pH 5. 5):	3. 87
ACD/BCF (pH 5. 5):	516. 59
ACD/KOC (pH 5. 5):	3045. 60
ACD/LogD (pH 7. 4):	3. 87
ACD/BCF (pH 7. 4):	516. 59
ACD/KOC (pH 7. 4):	3045. 60
Polar Surface Area:	9 Å <sup>2</sup>

Polarizability:  $18.9 \pm 0.5 \times 10^{-24} \text{ cm}^3$

Surface Tension:  $38.4 \pm 3.0 \text{ dyne/cm}$

Molar Volume:  $149.3 \pm 3.0 \text{ cm}^3$

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

EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 4. 01 Log Kow (Exper. database match) = 4. 11 Exper. Ref: Opperhuizen, A & Voors, PI (1987) Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 245. 41 (Adapted Stein & Brown method) Melting Pt (deg C): 43. 58 (Mean or Weighted MP) VP (mm Hg, 25 deg C): 0. 0193 (Modified Grain method) MP (exp database): 61. 5 deg CBP (exp database): 241 deg C Subcooled liquid VP: 0. 0422 mm Hg (25 deg C, Mod-Grain method) Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 11. 8 log Kow used: 4. 11 (expkow database) no-melting pt equation used Water Sol (Exper. database match) = 10 mg/L (20 deg C) Exper. Ref: PIRBAZARI, M ET AL (1992) Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 14. 329 mg/L Wat Sol (Exper. database match) = 10. 00 Exper. Ref: PIRBAZARI, M ET AL (1992) ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral Organics Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 30E-004 atm-m<sup>3</sup>/mole Group Method: 2. 68E-003 atm-m<sup>3</sup>/mole Henrys LC [VP/WSol estimate using EPI values]: 4. 551E-004 atm-m<sup>3</sup>/mole Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 11 (exp database) Log Kaw used: -2. 275 (HenryWin est) Log Koa (KOAWIN v1. 10 estimate): 6. 385 Log Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2315 Biowin2 (Non-Linear Model) : 0. 0220 Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 0539 (months ) Biowin4 (Primary Survey Model) : 3. 1237 (weeks ) MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3136 Biowin6 (MITI Non-Linear Model): 0. 0657 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 4631 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): 5. 63 Pa (0. 0422 mm Hg) Log Koa (Koawin est ): 6. 385 Kp (particle/gas partition coef. (m<sup>3</sup>/ug)): Mackay model : 5. 33E-007 Octanol/air (Koa) model: 5. 96E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 93E-005 Mackay model : 4. 27E-005 Octanol/air (Koa) model: 4. 77E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 4167 E-12 cm<sup>3</sup>/molecule-sec Half-Life = 7. 550 Days (12-hr day; 1. 5E6 OH/cm<sup>3</sup>) Half-Life = 90. 597 Hrs Ozone Reaction: No Ozone Reaction Estimation Fraction sorbed to airborne particulates (phi): 3. 1E-005 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 521. 4 Log Koc: 2. 717 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

= 2.465 (BCF = 291.5) log Kow used: 4.11 (expkow database) Volatilization from Water: Henry LC: 0.00268 atm-m<sup>3</sup>/mole (estimated by Group SAR Method) Half-Life from Model River: 1.802 hours Half-Life from Model Lake : 141.6 hours (5.9 days) Removal In Wastewater Treatment: Total removal: 64.61 percent Total biodegradation: 0.23 percent Total sludge adsorption: 28.28 percent Total to Air: 36.10 percent (using 10000 hr Bio P, A, S) Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 3.79 181 1000 Water 7.53 1.44e+003 1000 Soil 85.7 2.88e+003 1000 Sediment 2.95 1.3e+004 0 Persistence Time: 1.18e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop