

Furan C_4H_4O structure

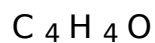


**ASSIGN
BUSTER**

Contents

- Retention Index (Linear):

Molecular



Formula

Average mass 68.074 Da

Density $0.9 \pm 0.1 \text{ g/cm}^3$ Boiling Point $31.4 \pm 9.0 \text{ }^\circ\text{C}$ at
760 mmHgFlash Point $-35.6 \pm 0.0 \text{ }^\circ\text{C}$

Molar

$$18.6 \pm 0.3 \text{ cm}^3$$

Refractivity

Polarizability $7.4 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface

$$24.8 \pm 3.0 \text{ dyne/cm}$$

Tension

Molar Volume $72.2 \pm 3.0 \text{ cm}^3$

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

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

- **Experimental Melting Point:**

-86 °C Alfa Aesar

-85.6 °C Oxford

University Chemical

Safety Data (No longer
updated) More details

-85.6 °C Jean-Claude

Bradley Open Melting

Point Dataset 15814,
20453

-85 °C Jean-Claude

Bradley Open Melting

Point Dataset 7253

-86 °C Alfa

Aesar A13102

- **Experimental Boiling Point:**

32-33 °C Alfa Aesar

31.4 °C Oxford

University Chemical

Safety Data (No longer

updated)More details

32-33 °CAlfa

AesarA13102

- **Experimental LogP:**

1. 34Egon

Willighagen[http://dx.](http://dx.doi.org/10.1021/ci050282s)

[doi. org/10.](http://dx.doi.org/10.1021/ci050282s)

[1021/ci050282s](http://dx.doi.org/10.1021/ci050282s)

- **Experimental Flash Point:**

-35 °CAlfa Aesar

-35 °COxford University

Chemical Safety Data

(No longer

updated)More details

-35 °CAlfa Aesar

-35 °F (-37. 2222

°C)Alfa AesarA13102

-35

°CLabNetworkLN00195

280

- **Experimental Gravity:**

20 g/mL Merck Millipore 3458

20 g/L Merck Millipore 3458,

820594

0.936 g/mL Alfa

Aesar A13102

- **Experimental Refraction Index:**

1.42 Alfa

Aesar A13102

- Miscellaneous

- **Appearance:**

colourless liquid Oxford

University Chemical

Safety Data (No longer

updated) More details

- **Stability:**

Stable. Substances to

be avoided include

strong oxidising

agents, acids,

peroxides and oxygen.

Highly flammable; can

form explosive

mixtures with air.

Oxford University

Chemical Safety Data

(No longer

updated) More details

- **Toxicity:**

IPR-RAT LD50 5 mg kg-

1 Oxford University

Chemical Safety Data

(No longer

updated) More details

- **Safety:**

3 Alfa Aesar A13102

45-12-19-20/22-38-

48/22-68-52/53 Alfa

Aesar A13102

53-45-61 Alfa

Aesar A13102

DangerAlfa

AesarA13102

DANGER: FLAMMABLE,

cancer risk, irritates

skin, eyes, lungsAlfa

AesarA13102

DANGER: FLAMMABLE,

irritates skin and

eyesAlfa AesarA13102

H224-H350-H341-

H373-H302-H332-

H315-H412-

EUH019Alfa

AesarA13102

P210-P260-P261-

P303+P361+P353-

P405-P501aAlfa

AesarA13102

Safety glasses, gloves,

good ventilation. Treat

as apotential

carcinogen. Oxford

University Chemical

Safety Data (No longer updated)More details

- Gas Chromatography

- **Retention Index (Kovats):**

553 (estimated with

error: 68)NIST

Spectramainlib_228308

, replib_19050

500 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0. 32

mm; Column length: 60

m; Column type:

Capillary; Start T: 100

C; CAS no: 110009;

Active phase: SPB-1;

Phase thickness: 0. 25

um; Data type: Kovats

RI; Authors: Misharina,

T. A.; Beletsky, I. V.;

Golovnya, R. V.,

Chromatographic and

IR characteristics of
methyl-, formyl-, and
acetyl-substituted
furans and thiophenes,
Russ. Chem. Bull.
(Engl. Transl.), 43(1),
1994, 64-69, In original
70-75.)NIST Spectranist
ri

498 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 2 m;
Column type: Packed;
Start T: 100 C; CAS no:
110009; Active phase:
SE-30; Substrate:
Gaschrom Q; Data
type: Kovats RI;
Authors: Winskowski, J.,
Gaschromatographisch
e Identifizierung von
Stoffen anhand von
Indexziffem und

unterschiedlichen
Detektoren,
Chromatographia,
17(3), 1983, 160-
165.)NIST Spectranist ri
485 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 6 m;
Column type: Packed;
Start T: 80 C; CAS no:
110009; Active phase:
SE-30; Carrier gas: He;
Substrate: Chromosorb
P; Data type: Kovats RI;
Authors: Viani, R.;
Muggler-Chavan, F.;
Reymond, D.; Egli, R.
H., 196. Sur la
composition de l'arome
de cafe, Helv. Chim.
Acta, 48(195-196),
1965, 1809-1815.)NIST

Spectranist ri

483 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column type: Packed;

Start T: 120 C; CAS no:

110009; Active phase:

Apiezon L; Substrate:

Celite 545; Data type:

Kovats RI; Authors:

Bogoslovsky, Yu. N.;

Anvaer, B. I.;

Vigdergauz, M. S.,

Chromatographic

constants in gas

chromatography (in

Russian), Standards

Publ. House, Moscow,

1978, 192.)NIST

Spectranist ri

492 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column type: Packed;

Start T: 160 C; CAS no:

110009; Active phase:

Apiezon L; Substrate:

Celite 545; Data type:

Kovats RI; Authors:

Bogoslovsky, Yu. N.;

Anvaer, B. I.;

Vigdergauz, M. S.,

Chromatographic

constants in gas

chromatography (in

Russian), Standards

Publ. House, Moscow,

1978, 192.)NIST

Spectranist ri

797 (Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

200 C; CAS no:

110009; Active phase:

PEG-2000; Carrier gas:
He; Substrate: Celite
545 (44-60 mesh);
Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.
VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-63.,
Program type: Ramp;
Column cl... (show
more)ass: Standard
polar; Column
diameter: 0.25 mm;
Column length: 60 m;
Column type: Capillary;
Heat rate: 3 K/min;
Start T: 40 C; End T:

190 C; Start time: 6
min; CAS no: 110009;
Active phase: DB-Wax;
Carrier gas: He; Data
type: Kovats RI;
Authors: Shimoda, M.;
Shibamoto, T., Isolation
and identification of
headspace volatiles
from brewed coffee
with an on-column
GC/MS method, J. Agric.
Food Chem., 38(3),
1990, 802-804.)NIST
Spectranist ri

786 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
length: 5. 5 m; Column
type: Packed; Heat
rate: 10 K/min; Start T:
70 C; End T: 175 C;
Start time: 9 min; CAS
no: 110009; Active

phase: PEG-20M;

Carrier gas: N2;

Substrate: Celite; Data

type: Kovats RI;

Authors: Galt, A. M.;

MacLeod, G.,

Headspace sampling of

cooked beef aroma

using Tenax GC, J.

Agric. Food Chem.,

32(1), 1984, 59-

64.)NIST Spectranist ri

779 (Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

152 C; CAS no:

110009; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska, M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines.

VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

790 (Program type:

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

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

179 C; CAS no:

110009; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

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

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

150 C; CAS no:

110009; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.
VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-
63.)NIST Spectranist ri

800 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
length: 3 m; Column
type: Packed; Start T:
180 C; CAS no:
110009; Active phase:
PEG-2000; Carrier gas:
He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska,

M.; Golender, L., Gas-

liquid chromatography

of some aliphatic and

heterocyclic mono- and

pollyfunctional amines.

VII. Retention indices of

amines in some polar

and unpolar stationary

phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

802 (Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

200 C; CAS no:

110009; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite
545 (44-60 mesh);
Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.
VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-
63.)NIST Spectranist ri

- **Retention Index (Lee):**

131. 1 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column length: 60 m;
Column type: Capillary;
CAS no: 110009; Active

phase: DB-5; Data
type: Lee RI; Authors:
Fuentes, M. J.; Font, R.;
Gomez-Rico, M. F.;
Martin-Gullon, I.,
Pyrolysis and
combustion of waste
lubricant oil from diesel
cars: Decomposition
and pollutants, J. Anal.
Appl. Pyrolysis, 79,
2007, 215-226.)NIST
Spectranist ri

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

500 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Capillary;
CAS no: 110009; Active
phase: OV-101; Data
type: Normal alkane RI;
Authors: Shibamoto, T.,
Retention Indices in
Essential Oil Analysis,

in Capillary Gas
Chromatography in
Essential Oil Analysis,
Sandra, P.; Bicchi, C.,
ed(s), Hutchig Verlag,
Heidelberg, New York,
1987, 259-274.,
Program type: Ramp;
Column cl... (show
more)ass: Standard
non-polar; Column
type: Capillary; CAS no:
110009; Active phase:
SE-30; Data type:
Normal alkane RI;
Authors: Vinogradov, B.
A., Production,
composition, properties
and application of
essential oils,
2004.)NIST Spectranist
ri

494. 7 (Program type:
Ramp; Column cl...
(show more)ass:

Standard non-polar;
Column diameter: 0.53
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 10
K/min; Start T: 40 C;
End T: 260 C; Start
time: 5 min; CAS no:
110009; Active phase:
DB-1; Carrier gas: He;
Phase thickness: 3 um;
Data type: Normal
alkane RI; Authors: J; W
Scientific, Solvent
Retention Data,
2003.)NIST Spectranist
ri

492 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0.32
mm; Column length: 50
m; Column type:
Capillary; Heat rate: 3

K/min; Start T: -30 C;
CAS no: 110009; Active
phase: DB-1; Phase
thickness: 1 um; Data
type: Normal alkane RI;
Authors: Barrefors, G.;
Bjorkqvist, S.; Ramnas,
O.; Petersson, G., Gas
chromatographic
separation of volatile
furans from birchwood
smoke, J. Chromatogr.
A, 753, 1996, 151-
155.)NIST Spectranist ri
522. 8 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 32
mm; Column length: 60
m; Column type:
Capillary; Heat rate: 2
K/min; Start T: 40 C;
End T: 240 C; CAS no:
110009; Active phase:

DB-5; Carrier gas: He;
Phase thickness: 0.25
um; Data type: Normal
alkane RI; Authors:
Moldoveanu, S. C.,
Pyrolysis GC/MS,
present and future
(recent past and
present needs), J.
Microcolumn Sep.,
13(3), 2001, 102-
125.)NIST Spectranist ri
495 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 3.2 m;
Column type: Packed;
Start T: 100 C; CAS no:
110009; Active phase:
Apiezon L; Data type:
Normal alkane RI;
Authors: Kavan, I.,
Analysis of odorants,
Sbornik Praci UVP, 26,

1973, 128-144, In
original 128-144.)NIST
Spectranist ri

760 (Program type:
Complex; Column...
(show more)class:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 50 m;
Column type: Capillary;
Description: 45 0C (15
min) ^ 3 0C/min -; 75
0C ^ 5 0C/min -; 180
0C (10 min); CAS no:
110009; Active phase:
Supelcowax 10; Carrier
gas: Helium; Phase
thickness: 0. 25 um;
Data type: Normal
alkane RI; Authors:
Soria, A. C.; Martinez-
Castro, I.; Sanz, J.,
Some aspects of
dynamic headspace
analysis of volatile

components in honey,
Foog Res. International,
41, 2008, 838-
848.)NIST Spectranist ri
786 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
type: Capillary; CAS no:
110009; Active phase:
Carbowax 20M; Data
type: Normal alkane RI;
Authors: Shibamoto, T.,
Retention Indices in
Essential Oil Analysis,
in Capillary Gas
Chromatography in
Essential Oil Analysis,
Sandra, P.; Bicchi, C.,
ed(s), Hutchig Verlag,
Heidelberg, New York,
1987, 259-274.,
Program type: Ramp;
Column cl... (show
more)ass: Standard

polar; Column type:
Capillary; CAS no:
110009; Active phase:
Carbowax 20M; Data
type: Normal alkane RI;
Authors: Vinogradov, B.
A., Production,
composition, properties
and application of
essential oils,
2004.)NIST Spectranist
ri

802. 9 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 53 mm;
Column length: 30 m;
Column type: Capillary;
Heat rate: 10 K/min;
Start T: 40 C; End T:
230 C; Start time: 7
min; CAS no: 110009;
Active phase: DB-Wax;
Carrier gas: He; Phase

thickness: 1 um; Data
type: Normal alkane RI;
Authors: J; W Scientific,
Solvent Retention
Data, 2003.)NIST
Spectranist ri

783 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 25 mm;
Column length: 25 m;
Column type: Capillary;
Heat rate: 5 K/min;
Start T: 40 C; End T:
200 C; End time: 20
min; Start time: 10
min; CAS no: 110009;
Active phase: CP-Wax
52CB; Carrier gas: N2;
Phase thickness: 0. 20
um; Data type: Normal
alkane RI; Authors:
Houeto, P.; Borron, S.
W.; Marliere, F.; Baud,

F. J.; Levillain, P.,
Development of a
method for measuring
volatile organic
compounds in the
blood of fire victims
using 'Purge and Trap'
gas chromatography,
Indoor+Built Environ.,
10, 2001, 62-69.)NIST
Spectranist ri

800 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0.25 mm;
Column length: 60 m;
Column type: Capillary;
Heat rate: 4 K/min;
Start T: 35 C; End T:
200 C; Start time: 10
min; CAS no: 110009;
Active phase:
Supelcowax-10; Carrier
gas: He; Phase

thickness: 0.25 um;

Data type: Normal

alkane RI; Authors:

Girard, B.; Durance, T.,

Headspace volatiles of

sockeye and pink

salmon as affected by

retort process, Food

Chem. Toxicol., 65(1),

2000, 34-39.)NIST

Spectranist ri

787.8 (Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

diameter: 0.02 in;

Column length: 50 ft;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 30 C; End T:

175 C; CAS no:

110009; Active phase:

Carbowax 20M; Carrier

gas: He; Data type:

Normal alkane RI;

Authors: Hruza, D. E.,
Sr.; van Praag, M.;
Heinsohn, H., Jr.,
Isolation and
identification of the
components of the tar
of hickory wood smoke,
J. Agric. Food Chem.,
22(1), 1974, 123-
126.)NIST Spectranist ri

- **Retention Index (Linear):**

500 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 32
mm; Column length: 50
m; Column type:
Capillary; Heat rate: 4
K/min; Start T: 50 C;
End T: 200 C; CAS no:
110009; Active phase:
OV-101; Carrier gas:
He; Phase thickness: 0.
5 um; Data type: Linear

RI; Authors: Misharina,
T. A.; Golovnya, R. V.;
Beletsky, I. V., Sorption
properties of
heterocyclic
compounds differing by
heteroatom in capillary
gas chromatography,
Russ. Chem. Bull.
(Engl. Transl.), 42(7),
1993, 1167-1170, In
original 1224-
1227.)NIST Spectranist
ri

801 (Program type:
Complex; Column...
(show more)class:
Standard polar; Column
diameter: 0.25 mm;
Column length: 30 m;
Column type: Capillary;
Description: 35C(8min)
=; 4C/min =; 60C =;
6C/min =; 160C=;
20C/min =;

200C(1min); CAS no:
110009; Active phase:
Supelcowax-10; Carrier
gas: He; Phase
thickness: 0.25 um;
Data type: Linear RI;
Authors: Bianchi, F.;
Careri, M.; Mangia, A.;
Musci, M., Retention
indices in the analysis
of food aroma volatile
compounds in
temperature-
programmed gas
chromatography:
Database creation and
evaluation of precision
and robustness, J. Sep.
Sci., 39, 2007, 563-
572.)NIST Spectranist ri
802 (Program type:
Complex; Column...
(show more)class:
Standard polar; Column
diameter: 0.25 mm;

Column length: 30 m;
Column type: Capillary;
Description: 35C(8min)
=; 4C/min =; 60C =;
6C/min =; 160C=;
20C/min =;
200C(1min); CAS no:
110009; Active phase:
Supelcowax-10; Carrier
gas: He; Phase
thickness: 0.25 um;
Data type: Linear RI;
Authors: Bianchi, F.;
Careri, M.; Mangia, A.;
Musci, M., Retention
indices in the analysis
of food aroma volatile
compounds in
temperature-
programmed gas
chromatography:
Database creation and
evaluation of precision
and robustness, J. Sep.
Sci., 39, 2007, 563-
572., Program type:

Ramp; Column cl...

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

Heat rate: 4 K/min;

Start T: 20 C; End T:

200 C; End time: 1 min;

Start time: 1 min; CAS

no: 110009; Active

phase: FFAP; Carrier

gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Ott, A.; Fay, L.

B.; Chaintreau, A.,

Determination and

origin of the aroma

impact compounds of

yogurt flavor, J. Agric.

Food Chem., 45, 1997,

850-858.)NIST

Spectranist ri

800 (Program type:

Ramp; Column cl...
(show more)ass:
Standard polar; Column
length: 3. 05 m;
Column type: Packed;
Heat rate: 8 K/min;
Start T: 40 C; End T:
200 C; End time: 60
min; Start time: 4 min;
CAS no: 110009; Active
phase: Carbowax 20M;
Substrate: Supelcoport;
Data type: Linear RI;
Authors: Peng, C. T.;
Yang, Z. C.; Ding, S. F.,
Prediction of retention
indexes. II. Structure-
retention index
relationship on polar
columns, J.
Chromatogr., 586,
1991, 85-112.)NIST
Spectranist ri

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

<https://assignbuster.com/furan-c4h4o-structure/>

Density:	0.9±0.1 g/cm ³
Boiling Point:	31.4±9.0 °C at 760 mmHg
Vapour Pressure:	605.2±0.1 mmHg at 25°C
Enthalpy of Vaporization:	27.1±0.0 kJ/mol
Flash Point:	-35.6±0.0 °C
Index of Refraction:	1.427
Molar Refractivity:	18.6±0.3 cm ³
#H bond acceptors:	1
#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	1.38
ACD/LogD (pH 5.5):	1.16
ACD/BCF (pH 5.5):	4.47
ACD/KOC (pH 5.5):	101.57
ACD/LogD (pH 7.4):	1.16

ACD/BCF (pH 7. 4):	4. 47
ACD/KOC (pH 7. 4):	101. 57
Polar Surface Area:	13 Å ²
Polarizability:	7. 4±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	24. 8±3. 0 dyne/cm
Molar Volume:	72. 2±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) = 1. 36
 Log Kow (Exper. database match) = 1. 34
 Exper. Ref: Hansch, C et al. (1995)
 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):
 Boiling Pt (deg C): 59. 30 (Adapted Stein & Brown method)
 Melting Pt (deg C): -87. 06 (Mean or Weighted MP)
 VP (mm Hg, 25 deg C): 596 (Mean VP of Antoine & Grain methods)
 MP (exp database): -85. 6 deg C
 CBP (exp database): 31. 5 deg C
 V (exp database): 6. 00E+02 mm Hg at 25 deg C
 Water Solubility Estimate from Log Kow (WSKOW v1. 41):
 Water Solubility at 25 deg C (mg/L): 9751
 log Kow used: 1. 34 (expkow database)
 no-melting pt equation used
 Water Sol (Exper. database match) = 1e+004 mg/L (25 deg C)
 Exper. Ref: VALVANI, SC ET AL. (1981)
 Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 12750 mg/L
 Wat Sol (Exper. database match) = 10000. 00
 Exper. Ref: VALVANI, SC ET AL. (1981)
 ECOSAR Class Program (ECOSAR v0. 99h):
 Class(es) found: Neutral Organics
 Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]:
 Bond Method : 5. 38E-003 atm-m³/mole
 Group Method: Incomplete
 Exper Database: 5. 40E-03 atm-m³/mole
 Henrys LC [VP/WSol estimate using EPI values]: 5. 475E-003 atm-m³/mole
 Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]:
 Log Kow used: 1. 34 (exp database)
 Log Kaw used: -0. 656 (exp database)
 Log Koa (KOAWIN v1. 10 estimate): 1. 996
 Log Koa (experimental database): None
 Probability of Rapid Biodegradation (BIOWIN v4. 10):
 Biowin1 (Linear Model) : 0. 7151
 Biowin2 (Non-Linear Model) : 0. 8851
 Expert Survey Biodegradation Results:
 Biowin3 (Ultimate Survey Model): 3. 0487 (weeks)
 Biowin4 (Primary Survey Model) : 3. 7495 (days-weeks)
 MITI Biodegradation Probability:
 Biowin5 (MITI Linear Model) : 0. 5425
 Biowin6 (MITI Non-Linear Model): 0. 7390
 Anaerobic Biodegradation Probability:
 Biowin7 (Anaerobic Linear Model): 0. 4544
 Ready Biodegradability Prediction: YES
 Hydrocarbon Biodegradation (BioHCwin v1. 01):
 Structure incompatible with

<https://assignbuster.com/furan-c4h4o-structure/>

current estimation method! Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 8E+004 Pa (600 mm Hg) Log Koa (Koawin est): 1. 996Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 75E-011 Octanol/air (Koa) model: 2. 43E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 35E-009 Mackay model : 3E-009 Octanol/air (Koa) model: 1. 95E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 40. 5000 E-12 cm3/molecule-sec Half-Life = 0. 264 Days (12-hr day; 1. 5E6 OH/cm3) Half-Life = 3. 169 Hrs Ozone Reaction: No Ozone Reaction Estimation Reaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 2. 18E-009 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 89. 71 Log Koc: 1. 953 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 = 0. 332 (BCF = 2. 147) log Kow used: 1. 34 (expkow database) Volatilization from Water: Henry LC: 0. 0054 atm-m3/mole (Henry experimental database) Half-Life from Model River: 0. 9314 hours (55. 89 min) Half-Life from Model Lake : 79. 35 hours (3. 306 days) Removal In Wastewater Treatment: Total removal: 68. 29 percent Total biodegradation: 0. 04 percent Total sludge adsorption: 0. 80 percent Total to Air: 67. 45 percent (using 10000 hr Bio P, A, S) Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 8. 23 6 1000 Water 81. 1 360 1000 Soil 10. 4 720 1000 Sediment 0. 179 3. 24e+003 0 Persistence Time: 78. 1 hr

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