

1-bromo-2-
methylpropane
c4h9br structure



**ASSIGN
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Contents

- Retention Index (Normal Alkane):

Molecular

C₄H₉Br

Formula

Average mass 137. 018 Da

Density 1. 3±0. 1 g/cm³

Boiling Point 90. 7±8. 0 °C at
760 mmHg

Flash Point 18. 3±0. 0 °C

Molar	
Refractivity	28. 3±0. 3 cm ³
Polarizability	11. 2±0. 5 10 ⁻²⁴ cm ³
Surface	
Tension	24. 6±3. 0 dyne/cm
Molar Volume	108. 1±3. 0 cm ³

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

- 118 °C Alfa Aesar

- 118 °C Jean-Claude

- Bradley Open Melting

- Point Dataset303

- 117 °C Jean-Claude

- Bradley Open Melting

Point Dataset13748

-119 °CJean-Claude

Bradley Open Melting

Point Dataset21186

-118 °CAlfa

AesarB23854

-117. 4 °CBiosynthJ-

504405

-119

°CLabNetworkLN00224

680

- **Experimental Boiling Point:**

90-92 °CAlfa Aesar

90-92 °CAlfa

AesarB23854

90. 7 °CBiosynthJ-

504405

90-92

°CLabNetworkLN00224

680

- **Experimental Flash Point:**

18 °C Alfa Aesar

18 °C Alfa Aesar

18 °F (-7.7778 °C) Alfa

AesarB23854

18

°C LabNetworkLN00224

680

- **Experimental Gravity:**

20 g/mL Merck

Millipore1259

20 g/L Merck

Millipore1259, 801549

1.255 g/mL Alfa

AesarB23854

18.3 g/mL BiosynthJ-

504405

- **Experimental Refraction Index:**

1.435 Alfa

AesarB23854

- **Experimental Solubility:**

-2. 43Egon

Willighagenhttp://dx.

doi. org/10.

1021/ci050282s

Slightly soluble in

water. Miscible with

alcohol, etherAlfa

AesarB23854

- Miscellaneous

- **Safety:**

11-36/37/38Alfa

AesarB23854

3Alfa AesarB23854

7-26-33-37-43Alfa

AesarB23854

DangerAlfa

AesarB23854

DANGER: FLAMMABLE,

irritates skin, eyes,

lungsAlfa AesarB23854

H225-H315-H319-

H335Alfa AesarB23854

P210-P261-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

AesarB23854

- Gas Chromatography

- **Retention Index (Kovats):**

651 (estimated with

error: 62)NIST

Spectramainlib_227727

, replib_21078,

replib_58847,

replib_163852

666 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0.25

mm; Column length: 50

ft; Column type:

Packed; Start T: 27 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: He;
Substrate: Chromosorb
P; Data type: Kovats RI;
Authors: Hively, R. A.;
Hinton, R. E., Variation
of the retention index
with temperature on
squalane substrates, J.
Gas Chromatogr., 6,
1968, 203-217.)NIST
Spectranist ri

671 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 50
ft; Column type:
Packed; Start T: 49 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: He;

Substrate: Chromosorb
P; Data type: Kovats RI;
Authors: Hively, R. A.;
Hinton, R. E., Variation
of the retention index
with temperature on
squalane substrates, J.
Gas Chromatogr., 6,
1968, 203-217.)NIST
Spectranist ri

676 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 50
ft; Column type:
Packed; Start T: 67 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: He;
Substrate: Chromosorb
P; Data type: Kovats RI;
Authors: Hively, R. A.;
Hinton, R. E., Variation

of the retention index
with temperature on
squalane substrates, J.
Gas Chromatogr., 6,
1968, 203-217.,
Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 1. 5 m;
Column type: Packed;
Start T: 78 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
Mixture; Substrate:
Celite; Data type:
Kovats RI; Authors:
Adlard, E. R.; Evans, M.
B.; Butlin, A. G.; Evans,
R. S.; Hill, R.; Huber, J.
F. K.; Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-

committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column length:
1. 8 m; Column type:
Packed; Start T: 78 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: N2;
Substrate: Celite; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-

committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

680 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 50
ft; Column type:
Packed; Start T: 86 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: He;
Substrate: Chromosorb
P; Data type: Kovats RI;
Authors: Hively, R. A.;
Hinton, R. E., Variation
of the retention index
with temperature on
squalane substrates, J.
Gas Chromatogr., 6,

1968, 203-217.,

Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 1. 5 m;

Column type: Packed;

Start T: 100 C; CAS no:

78773; Active phase:

Squalane; Carrier gas:

Ar; Substrate: Celite;

Data type: Kovats RI;

Authors: Adlard, E. R.;

Evans, M. B.; Butlin, A.

G.; Evans, R. S.; Hill, R.;

Huber, J. F. K.;

Littlewood, A. B.;

McCambley, W. G.;

Smith, J. F.; Swanton,

W. T.; Swoboda, P. A.

T., Recommendations

of the data sub-

committee for the

publication of retention

data, J. Gas

Chromatogr., , 1965,

298-302.)NIST

Spectranist ri

672 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 1. 5 m;

Column type: Packed;

Start T: 65 C; CAS no:

78773; Active phase:

Squalane; Carrier gas:

Ar; Substrate: Celite;

Data type: Kovats RI;

Authors: Adlard, E. R.;

Evans, M. B.; Butlin, A.

G.; Evans, R. S.; Hill, R.;

Huber, J. F. K.;

Littlewood, A. B.;

McCambley, W. G.;

Smith, J. F.; Swanton,

W. T.; Swoboda, P. A.

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committee for the

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data, J. Gas

Chromatogr., , 1965,

298-302.)NIST

Spectranist ri

673 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 1. 5 m;

Column type: Packed;

Start T: 65 C; CAS no:

78773; Active phase:

Squalane; Carrier gas:

Mixture; Substrate:

Celite; Data type:

Kovats RI; Authors:

Adlard, E. R.; Evans, M.

B.; Butlin, A. G.; Evans,

R. S.; Hill, R.; Huber, J.

F. K.; Littlewood, A. B.;

McCambley, W. G.;

Smith, J. F.; Swanton,

W. T.; Swoboda, P. A.

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data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column length:
1. 8 m; Column type:
Packed; Start T: 65 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: N2;
Substrate: Celite; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-

committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

674 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 1. 2 m;
Column type: Packed;
Start T: 65 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
Ar; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.

T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column type:
Packed; Start T: 65 C;
CAS no: 78773; Active
phase: Squalane; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-
committee for the

publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

675 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 1. 5 m;
Column type: Packed;
Start T: 78 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
Ar; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations

of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

677 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 0. 9 m;
Column type: Packed;
Start T: 65 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
He; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,

W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column length:
1. 2 m; Column type:
Packed; Start T: 78 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: Ar;
Substrate: Celite; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
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data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column type:
Packed; Start T: 78 C;
CAS no: 78773; Active
phase: Squalane; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
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data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

679 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 0. 9 m;
Column type: Packed;
Start T: 78 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
He; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.

T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302., Program
type: Isothermal; Col...
(show more)umn class:
Semi-standard non-
polar; Column length:
1. 5 m; Column type:
Packed; Start T: 100 C;
CAS no: 78773; Active
phase: Squalane;
Carrier gas: Mixture;
Substrate: Celite; Data
type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.

T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

681 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 1. 8 m;
Column type: Packed;
Start T: 100 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
N2; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;
McCambley, W. G.;

Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

682 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Packed;
Start T: 100 C; CAS no:
78773; Active phase:
Squalane; Data type:
Kovats RI; Authors:
Adlard, E. R.; Evans, M.
B.; Butlin, A. G.; Evans,
R. S.; Hill, R.; Huber, J.
F. K.; Littlewood, A. B.;
McCambley, W. G.;
Smith, J. F.; Swanton,

W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

686 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 0. 9 m;
Column type: Packed;
Start T: 100 C; CAS no:
78773; Active phase:
Squalane; Carrier gas:
He; Substrate: Celite;
Data type: Kovats RI;
Authors: Adlard, E. R.;
Evans, M. B.; Butlin, A.
G.; Evans, R. S.; Hill, R.;
Huber, J. F. K.;
Littlewood, A. B.;

McCambley, W. G.;
Smith, J. F.; Swanton,
W. T.; Swoboda, P. A.
T., Recommendations
of the data sub-
committee for the
publication of retention
data, J. Gas
Chromatogr., , 1965,
298-302.)NIST
Spectranist ri

699 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Packed;
Start T: 70 C; CAS no:
78773; Active phase:
Apiezon L; Substrate:
Celite (40: 60
Gewichtsverhältnis);
Data type: Kovats RI;
Authors: von Kovats,
E., 206. Gas-
chromatographische

Charakterisierung

organischer

Verbindungen. Teil 1:

Retentionsindices

aliphatischer

Halogenide, Alkohole,

Aldehyde und Ketone,

Helv. Chim. Acta,

41(7), 1958, 1915-

1932.)NIST Spectranist

ri

711 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column type: Packed;

Start T: 130 C; CAS no:

78773; Active phase:

Apiezon L; Substrate:

Celite (40: 60

Gewichtsverhältnis);

Data type: Kovats RI;

Authors: von Kovats,

E., 206. Gas-

chromatographische

Charakterisierung

organischer

Verbindungen. Teil 1:

Retentionsindices

aliphatischer

Halogenide, Alkohole,

Aldehyde und Ketone,

Helv. Chim. Acta,

41(7), 1958, 1915-

1932.)NIST Spectranist

ri

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

677 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Capillary;

CAS no: 78773; Active

phase: Methyl Silicone;

Data type: Normal

alkane RI; Authors:

Zenkevich, I. G.;

Marinichev, A. N.,

Comparison of

Topological and

Dynamics Molecular
Characteristics for
Precalculation of
Chromatographic
Retention Parameters
of Organic Compounds
(in Russian), Zh. Struct.
Khim., 42(5), 2001,
893-902, In original
893-902.)NIST
Spectranist ri

677. 2 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 25
mm; Column length: 50
m; Column type:
Capillary; CAS no:
78773; Active phase:
Silicone oil; Carrier gas:
N2; Data type: Normal
alkane RI; Authors:
Hepburn, D. R.;
Hudson, H. R., Gas

chromatography of
alkyl halides on a
silicone oil capillary
column, J. Chromatogr.,
103, 1975, 166-
169.)NIST Spectranist ri

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

Density:	1.3 ± 0.1 g/cm ³
Boiling Point:	90.7 ± 8.0 °C at 760 mmHg
Vapour Pressure:	62.9 ± 0.2 mmHg at 25°C
Enthalpy of Vaporization:	31.3 ± 0.0 kJ/mol
Flash Point:	18.3 ± 0.0 °C
Index of Refraction:	1.436
Molar Refractivity:	28.3 ± 0.3 cm ³
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0

ACD/LogP:	2. 56
ACD/LogD (pH 5. 5):	2. 46
ACD/BCF (pH 5. 5):	43. 32
ACD/KOC (pH 5. 5):	516. 61
ACD/LogD (pH 7. 4):	2. 46
ACD/BCF (pH 7. 4):	43. 32
ACD/KOC (pH 7. 4):	516. 61
Polar Surface Area:	0 Å ²
Polarizability:	11. 2±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	24. 6±3. 0 dyne/cm
Molar Volume:	108. 1±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) = 2. 58
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):
Boiling Pt (deg C): 87. 38 (Adapted Stein & Brown method) Melting Pt (deg C): -78. 08 (Mean or Weighted MP)
VP (mm Hg, 25 deg C): 62 (Mean VP of Antoine & Grain methods) MP (exp database): -119 deg C
CBP (exp database): 91. 1 deg C
Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 543. 9
log Kow used: 2. 58 (estimated) no-melting pt equation used
Water Sol (Exper. database match) = 507 mg/L (18 deg C) Exper. Ref:

<https://assignbuster.com/1-bromo-2-methylpropane-c4h9br-structure/>

YALKOWSKY, SH & DANNENFELSER, RM (1992) Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1285.6 mg/L Wat Sol (Exper. database match) = 507.00 Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992) ECOSAR Class Program (ECOSAR v0.99h): Class(es) found: Neutral Organics Henrys Law Constant (25 deg C) [HENRYWIN v3.10]: Bond Method : 1.99E-002 atm-m³/mole Group Method: 1.94E-002 atm-m³/mole Henrys LC [VP/WSol estimate using EPI values]: 2.055E-002 atm-m³/mole Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]: Log Kow used: 2.58 (KowWin est) Log Kaw used: -0.090 (HenryWin est) Log Koa (KOAWIN v1.10 estimate): 2.670 Log Koa (experimental database): None Probability of Rapid Biodegradation (BIOWIN v4.10): Biowin1 (Linear Model) : 0.6361 Biowin2 (Non-Linear Model) : 0.0329 Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2.9253 (weeks) Biowin4 (Primary Survey Model) : 3.6854 (days-weeks) MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0.4008 Biowin6 (MITI Non-Linear Model): 0.1656 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0.8962 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): 7.93E+003 Pa (59.5 mm Hg) Log Koa (Koawin est) : 2.670 Kp (particle/gas partition coef. (m³/ug)): Mackay model : 3.78E-010 Octanol/air (Koa) model: 1.15E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1.37E-008 Mackay model : 3.03E-008 Octanol/air (Koa) model: 9.19E-009 Atmospheric Oxidation (25 deg C) [AopWin v1.92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1.5486 E-12 cm³/mole-sec Half-Life = 6.907 Days (12-hr day; 1.5E6 OH/cm³) Half-Life = 82.881 Hrs Ozone Reaction: No Ozone Reaction Estimation Fraction sorbed to airborne particulates (phi): 2.2E-008 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1.66): Koc : 67.7 Log Koc: 1.831 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]: Total Kb for pH > 8 at 25 deg C : 1.203E-010 L/mol-sec Kb Half-Life at pH 8: 1.826E+008 years Kb Half-Life at pH 7: 1.826E+009 years Bioaccumulation Estimates from Log Kow (BCFWIN v2.17): Log BCF from regression-based method = 1.283 (BCF = 19.2) log Kow used: 2.58 (estimated) Volatilization from Water: Henry LC: 0.0194 atm-m³/mole (estimated by Group SAR Method) Half-Life from Model River: 1.23 hours Half-Life from Model Lake : 111.6 hours (4.649 days) Removal In Wastewater Treatment: Total removal: 88.39 percent Total biodegradation: 0.03 percent Total sludge adsorption: 1.38 percent Total to Air: 86.98 percent (using 10000 hr Bio P, A, S) Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 41.6 166 1000 Water 45.6 360 1000 Soil 12.4 720 1000 Sediment 0.362 3.24E+003 0 Persistence Time: 136 hr

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