

Nikethamide

c10h14n2o structure



Contents

- Retention Index (Linear):

Molecular Formula	$C_{10}H_{14}N_2O$
Average mass	178.231 Da
Density	$1.0 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$298.0 \pm 0.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$141.1 \pm 20.4 \text{ }^\circ\text{C}$
Molar Refractivity	$52.0 \pm 0.3 \text{ cm}^3$
Polarizability	$20.6 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$40.6 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$171.0 \pm 3.0 \text{ cm}^3$

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

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

- **Experimental Melting Point:**

24-26 °COxford

University Chemical

Safety Data (No longer
updated)More details

25 °CJean-Claude

Bradley Open Melting

Point Dataset15953,

21485

- **Experimental Boiling Point:**

296 °COxford University

Chemical Safety Data

(No longer updated)More
details

- **Experimental Flash Point:**

22 °CTCID0514

112 °COxford University

Chemical Safety Data

(No longer updated)More

details

- Miscellaneous

- **Appearance:**

light yellow viscous

liquidOxford University

Chemical Safety Data

(No longer updated)More

details

- **Toxicity:**

IVN-RAT LD50 191 mg

kg-1, SCU-RAT LD50 240

mg kg-1, ORL-MUS LD50

188 mg kg-1, ORL-RBT

LD50 650 mg kg-

1Oxford University

Chemical Safety Data

(No longer updated)More

details

- **Safety:**

DangerBiosynthW-

105333

GHS06BiosynthW-

105333

H301; H315; H319;

H335BiosynthW-105333

P261; P301+P310;

P305+P351+P338Biosyn

thW-105333

Safety glasses. Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Target Organs:**

GABARTargetMolT004

8

- **Bio Activity:**

GABARTargetMolT0048

NeuroscienceTargetMolT

0048

- Gas Chromatography

- **Retention Index (Kovats):**

1386 (estimated with

error: 83)NIST

Spectramainlib_291418,

replib_42285,

replib_234082

1520 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column length: 2 m;

Column type: Packed;

Start T: 140 C; CAS no:

59267; Active phase: SE-

30; Carrier gas: N2;

Substrate: 1% se-30 on

Anachrom ABS(80-

100mesh); Data type:

Kovats RI; Authors:

Musumarra, G.; Scarlata,

G.; Romano, G.;

Cappello, G.; Clementi,

S.; Giuliatti, G.,

Qualitative organic

analysis. Part 2.

Identification of drugs by

principal components

analysis of standardized
TLC data in four eluent
systems and of retention
indices on SE 30, J. Anal.
Toxicol., 11, 1987, 154-
163.)NIST Spectranist ri

1515 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 49
mm; Column length: 25
m; Column type:
Capillary; Heat rate: 8
K/min; Start T: 100 C;
End T: 275 C; End time:
15 min; Start time: 2
min; CAS no: 59267;
Active phase: SE-30;
Phase thickness: 1. 14
um; Data type: Kovats
RI; Authors: Schepers,
P.; Wijsbeek, J.; Franke,
J. P.; de Zeeuw, R. A.,
Applicability of capillary

gas chromatography to
substance identification
in toxicology by means
of retention indices, J.
Forensic Sci., 27(1),
1982, 49-60.)NIST
Spectranist ri

1536 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 22
mm; Column length: 12
m; Column type:
Capillary; Heat rate: 8
K/min; Start T: 120 C;
End T: 300 C; End time:
12 min; Start time: 2
min; CAS no: 59267;
Active phase: SE-30;
Carrier gas: He; Phase
thickness: 0. 45 um;
Data type: Kovats RI;
Authors: Schepers, P.;
Wijsbeek, J.; Franke, J.

P.; de Zeeuw, R. A.,
Applicability of capillary
gas chromatography to
substance identification
in toxicology by means
of retention indices, J.
Forensic Sci., 27(1),
1982, 49-60.)NIST
Spectranist ri

1530 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 6 ft;
Column type: Packed;
CAS no: 59267; Active
phase: OV-101; Carrier
gas: N2; Substrate:
Chromosorb W; Data
type: Kovats RI; Authors:
McLinden, V. J.;
Stenhouse, A. M., A
chromatography system
for drug identification,
Forensic Sci. Int., 13,

1979, 71-79.)NIST

Spectranist ri

1503 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column type: Packed;

Start T: 150 C; CAS no:

59267; Active phase:

OV-101; Substrate: Gas

Chrom Q (80-100 mesh);

Data type: Kovats RI;

Authors: Delley, R.;

Friedrich, K., System CG

72 von bevorzugten

Trennflüssigkeiten für

die Gas-

Chromatographie,

Chromatographia,

10(10), 1977, 593-

600.)NIST Spectranist ri

1500 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;
Column length: 2 m;
Column type: Packed;
CAS no: 59267; Active
phase: SE-30; Data type:
Kovats RI; Authors:
Moffat, A. C.; Stead, A.
H.; Smalldon, K. W.,
Optimum use of paper,
thin-layer and gas-liquid
chromatography for the
identification of basic
drugs. III. Gas-liquid
chromatography, J.
Chromatogr., 90, 1974,
19-33.)NIST Spectranist
ri

1487 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Packed;
Start T: 160 C; CAS no:
59267; Active phase:
Apiezon L; Data type:

Kovats RI; Authors:
Huber, J. F. K.; Kenndler,
E.; Reich, G.,
Quantitation of the
Information Content of
Multi-Dimensional Gas
Chromatography and
Low- Resolution Mass
Spectrometry in the
Identification of Doping
Drugs, J. Chromatogr.,
172, 1979, 15-30.)NIST
Spectranist ri

1486 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Packed;
Start T: 160 C; CAS no:
59267; Active phase:
Apiezon L; Substrate:
Chromosorb W; Data
type: Kovats RI; Authors:
Donike, M.; Stratmann,
D., Gas-

chromatographische
identifizierung von
stimulantien der
phenylathylaminreihe
mit hilfe der retentions-
indices, Z. Anal. Chem.,
279(2), 1976, 129-
131.)NIST Spectranist ri

2319 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
type: Packed; Start T:
180 C; CAS no: 59267;
Active phase: PEG-20M;
Carrier gas: N2; Data
type: Kovats RI; Authors:
Huber, J. F. K.; Kenndler,
E.; Reich, G.,

Quantitation of the
Information Content of
Multi-Dimensional Gas
Chromatography and
Low- Resolution Mass
Spectrometry in the

Identification of Doping

Drugs, J. Chromatogr.,

172, 1979, 15-30.,

Program type:

Isothermal; Col... (show

more)umn class:

Standard polar; Column

type: Packed; Start T:

180 C; CAS no: 59267;

Active phase: PEG-20M;

Substrate: Chromosorb

W; Data type: Kovats RI;

Authors: Donike, M.;

Stratmann, D., Gas-

chromatographische

identifizierung von

stimulantien der

phenylathylaminreihe

mit hilfe der retnetions-

indices, Z. Anal. Chem.,

279(2), 1976, 129-

131.)NIST Spectranist ri

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

1505 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 2 m;

Column type: Packed;

Heat rate: 2.5 K/min;

Start T: 120 C; End T:

200 C; CAS no: 59267;

Active phase: SE-30;

Substrate: Gas Chrom P;

Data type: Normal

alkane RI; Authors:

Marozzi, E.; Gambaro,

V.; Saligari, E.; Mariani,

R.; Lodi, F., Use of the

retention index in gas

chromatographic studies

of drugs, J. Anal.

Toxicol., 6, 1982, 185-

192.)NIST Spectranist ri

1510 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 2 m;

Column type: Packed;

Heat rate: 2.5 K/min;
Start T: 120 C; End T:
200 C; CAS no: 59267;
Active phase: OV-1;
Substrate: Gas Chrom P;
Data type: Normal
alkane RI; Authors:
Marozzi, E.; Gambaro,
V.; Saligari, E.; Mariani,
R.; Lodi, F., Use of the
retention index in gas
chromatographic studies
of drugs, J. Anal.
Toxicol., 6, 1982, 185-
192.)NIST Spectranist ri
1525 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Other; CAS
no: 59267; Active phase:
Methyl Silicone; Data
type: Normal alkane RI;
Authors: Ardrey, R. E.;
Moffat, A. C., Gas-liquid

chromatographic
retention indices of 1318
substances of
toxicological interest on
SE-30 or OV-1 stationary
phase, J. Chromatogr.,
220, 1981, 195-
252.)NIST Spectranist ri
1528. 7 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0. 2
mm; Column length: 12.
5 m; Column type:
Capillary; Heat rate: 25
K/min; Start T: 75 C; End
T: 320 C; End time: 2
min; CAS no: 59267;
Active phase: Ultra-2;
Phase thickness: 0. 11
um; Data type: Normal
alkane RI; Authors:
Hemmersbach, P.; de la
Torre, R., Review.

Stimulants, narcotics
and . beta.-blockers: 25
years of development in
analytical techniques for
doping control, J.

Chromatogr. B, 687,
1996, 221-238.)NIST

Spectranist ri

1457 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 150 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,

Chromatographic
screening for drugs of
abuse using capillary
columds. II. Peak
identification on support
coated open tubular

columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1459 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 150 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,
Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system

stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1462 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 150 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,

Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),

1973, 293-300.)NIST

Spectranist ri

1463 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column type: Capillary;

Start T: 150 C; CAS no:

59267; Active phase:

Apieson L / KOH; Data

type: Normal alkane RI;

Authors: Caddy, B.; Fish,

F.; Scott, D.,

Chromatographic

screening for drugs of

abuse using capillary

columns. II. Peak

identification on support

coated open tubular

columns for a series of

central nervous system

stimulating drugs,

Chromatographia, 6(7),

1973, 293-300.)NIST

Spectranist ri

1464 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
CAS no: 59267; Active
phase: Apieson L / KOH;
Data type: Normal
alkane RI; Authors:
Caddy, B.; Fish, F.; Scott,
D., Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1466 (Program type:
Isothermal; Col... (show
more)umn class: Semi-

standard non-polar;
Column type: Capillary;
Start T: 150 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,
Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1470 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;

Start T: 150 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,

Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1503 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 190 C; CAS no:
59267; Active phase:

Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,
Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1506 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 190 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;

Authors: Caddy, B.; Fish,
F.; Scott, D.,

Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

1511 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column type: Capillary;
Start T: 190 C; CAS no:
59267; Active phase:
Apieson L / KOH; Data
type: Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,

Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

2375 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
type: Capillary; Start T:
190 C; CAS no: 59267;
Active phase: Carbowax
20M / KOH; Data type:
Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,
Chromatographic
screening for drugs of

abuse using capillary
columns. II. Peak
identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

2386 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
type: Capillary; Start T:
190 C; CAS no: 59267;
Active phase: Carbowax
20M / KOH; Data type:
Normal alkane RI;
Authors: Caddy, B.; Fish,
F.; Scott, D.,
Chromatographic
screening for drugs of
abuse using capillary
columns. II. Peak

identification on support
coated open tubular
columns for a series of
central nervous system
stimulating drugs,
Chromatographia, 6(7),
1973, 293-300.)NIST
Spectranist ri

- **Retention Index (Linear):**

1497 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 25
mm; Column length: 15
m; Column type:
Capillary; Heat rate: 8
K/min; Start T: 120 C;
End T: 280 C; End time:
5 min; CAS no: 59267;
Active phase: DB-1;
Carrier gas: He; Phase
thickness: 0. 25 um;
Data type: Linear RI;
Authors: Perrigo, B. J.;

Ballantyne, D. J.; Peel, H. W., Considerations in developing a data base for drugs on a DBI capillary column, J. Can. Soc. Forensic Sci., 17(2), 1984, 41-49., Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 15 m; Column type: Capillary; Heat rate: 8 K/min; Start T: 120 C; End T: 280 C; End time: 5 min; CAS no: 59267; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Perrigo, B. J.; Peel, H. W.; Ballantyne, D. J., Use of Dual-Column Fused-Silica Capillary Gas Chromatography in

Combination with
Detector Response
Factors for Analytical
Toxicology., J.
Chromatogr., 341, 1985,
81-88.)NIST Spectranist
ri

1494 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 25
mm; Column length: 15
m; Column type:
Capillary; Heat rate: 5
K/min; Start T: 120 C;
End T: 280 C; End time:
5 min; CAS no: 59267;
Active phase: DB-1;
Carrier gas: He; Phase
thickness: 0. 25 um;
Data type: Linear RI;
Authors: Perrigo, B. J.;
Ballantyne, D. J.; Peel, H.
W., Condierations in

developing a data base
for drugs on a DBI
capillary column, J. Can.
Soc. Forensic Sci., 17(2),
1984, 41-49.)NIST
Spectranist ri

1500 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0.25
mm; Column length: 15
m; Column type:
Capillary; Heat rate: 12
K/min; Start T: 120 C;
End T: 280 C; End time:
5 min; CAS no: 59267;
Active phase: DB-1;
Carrier gas: He; Phase
thickness: 0.25 um;
Data type: Linear RI;
Authors: Perrigo, B. J.;
Ballantyne, D. J.; Peel, H.
W., Condierations in
developing a data base

for drugs on a DBI
capillary column, J. Can.
Soc. Forensic Sci., 17(2),
1984, 41-49., Program
type: Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 25
mm; Column length: 15
m; Column type:
Capillary; Heat rate: 15
K/min; Start T: 120 C;
End T: 280 C; End time:
5 min; CAS no: 59267;
Active phase: DB-1;
Carrier gas: He; Phase
thickness: 0. 25 um;
Data type: Linear RI;
Authors: Perrigo, B. J.;
Ballantyne, D. J.; Peel, H.
W., Condierations in
developing a data base
for drugs on a DBI
capillary column, J. Can.
Soc. Forensic Sci., 17(2),
1984, 41-49., Program

type: Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 1. 8 m;

Column type: Packed;

Heat rate: 8 K/min; Start

T: 130 C; End T: 290 C;

End time: 8 min; Start

time: 2 min; CAS no:

59267; Active phase: SE-

30; Carrier gas: N2;

Substrate: Chromosorb

W; Data type: Linear RI;

Authors: Perrigo, B. J.;

Peel, H. W., The use of

retention indices and

temperature-

programmed gas

chromatography in

analytical toxicology, J.

Chromatogr. Sci., 19,

1981, 219-226.)NIST

Spectranist ri

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

<https://assignbuster.com/nikethamide-c10h14n2o-structure/>

Density:	1.0±0.1 g/cm ³
Boiling Point:	298.0±0.0 °C at 760 mmHg
Vapour Pressure:	0.0±0.6 mmHg at 25°C
Enthalpy of Vaporization:	53.8±3.0 kJ/mol
Flash Point:	141.1±20.4 °C
Index of Refraction:	1.520
Molar Refractivity:	52.0±0.3 cm ³
#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	0.33
ACD/LogD (pH 5.5):	0.54
ACD/BCF (pH 5.5):	1.51
ACD/KOC (pH 5.5):	46.52

ACD/LogD (pH 7. 4):	0. 54
ACD/BCF (pH 7. 4):	1. 52
ACD/KOC (pH 7. 4):	47. 06
Polar Surface Area:	33 Å ²
Polarizability:	20. 6±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	40. 6±3. 0 dyne/cm
Molar Volume:	171. 0±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) = 0. 52Log Kow (Exper. database match) = 0. 33Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 300. 45 (Adapted Stein & Brown method)Melting Pt (deg C): 88. 39 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00217 (Modified Grain method)MP (exp database): 25 deg CBP (exp database): 298 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 1438log Kow used: 0. 33 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1e+006 mg/L (25 deg C)Exper. Ref: MERCK (1989)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 98958 mg/LWat Sol (Exper. database match) = 1000000. 00Exper. Ref: MERCK (1989)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 46E-011 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 539E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 33 (exp database)Log Kaw used: -8. 998 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 328Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7183Biowin2 (Non-Linear Model) : 0. 8221Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5369 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7773 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4076Biowin6 (MITI Non-Linear Model): 0. 3067Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4204Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 289 Pa (0. 00217 mm Hg)Log Koa (Koawin

<https://assignbuster.com/nikethamide-c10h14n2o-structure/>

est): 9. 328Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 04E-005 Octanol/air (Koa) model: 0. 000522 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 000374 Mackay model : 0. 000829 Octanol/air (Koa) model: 0. 0401 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 23. 3306 E-12 cm3/molecule-secHalf-Life = 0. 458 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 501 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000602 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 331. 3Log Koc: 2. 520 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. 500 (BCF = 3. 162)log Kow used: 0. 33 (expkow database)Volatilization from Water: Henry LC: 2. 46E-011 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 3. 177E+007 hours (1. 324E+006 days)Half-Life from Model Lake : 3. 466E+008 hours (1. 444E+007 days)Removal In Wastewater Treatment: Total removal: 1. 86 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 000338 11 1000 Water 45 900 1000 Soil 54. 9 1. 8e+003 1000 Sediment 0. 0883 8. 1e+003 0 Persistence Time: 991 hr

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