

Ethyl 3,5-  
dinitrobenzoate  
c<sub>9</sub>h<sub>8</sub>n<sub>2</sub>o<sub>6</sub> structure



**ASSIGN  
BUSTER**

## Contents

- Retention Index (Linear):

Molecular Formula	$C_9H_8N_2O_6$
Average mass	240.170 Da
Density	$1.4 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$367.1 \pm 22.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$171.8 \pm 24.3 \text{ }^\circ\text{C}$
Molar Refractivity	$55.8 \pm 0.3 \text{ cm}^3$
Polarizability	$22.1 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$58.3 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$167.5 \pm 3.0 \text{ cm}^3$

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

- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

91-92 °C Alfa Aesar

94 °C Jean-Claude Bradley Open Melting Point

Dataset23389

92 °C Jean-Claude Bradley Open Melting Point

Dataset7078

91-92 °C Alfa Aesar B21582

94-95 °C Indofine [CS-532]

- Miscellaneous

- **Safety:**

CAUTION: May irritate eyes, skin, and respiratory tract Alfa

Aesar B21582

- Gas Chromatography

- **Retention Index (Kovats):**

1951 (estimated with error: 89) NIST Spectra mainlib\_117877, replib\_1929  
replib\_375615

1757 (Program type: Isothermal; Col... (show more) umn class: Standard  
polar; Column diameter: 0.33 mm; Column length: 25 m; Column type: C

Start T: 160 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Da

Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analysis XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic, 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr. 356, 1986, 285-299.)NIST Spectranist ri

1760 (Program type: Isothermal; Column class: Standard polar; Column diameter: 0.33 mm; Column length: 25 m; Column type: Capillary; Start T: 180 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data

Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analysis XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic, 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr. 356, 1986, 285-299.)NIST Spectranist ri

1767 (Program type: Isothermal; Column class: Standard polar; Column diameter: 0.33 mm; Column length: 25 m; Column type: Capillary; Start T: 200 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data

Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analysis XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic, 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr. 356, 1986, 285-299.)NIST Spectranist ri

1781 (Program type: Isothermal; Column class: Standard polar; Column diameter: 0.33 mm; Column length: 25 m; Column type: Capillary; Start T: 220 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data

Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analysis XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic, 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr. 356, 1986, 285-299.)NIST Spectranist ri

356, 1986, 285-299.)NIST Spectranist ri

1810 (Program type: Isothermal; Col... (show more)umn class: Standard  
polar; Column diameter: 0. 33 mm; Column length: 25 m; Column type: C  
Start T: 240 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Da  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitroben  
3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chro  
356, 1986, 285-299.)NIST Spectranist ri

1752 (Program type: Isothermal; Col... (show more)umn class: Standard  
polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: C  
Start T: 140 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Da  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromat  
360, 1986, 63-78.)NIST Spectranist ri

1762 (Program type: Isothermal; Col... (show more)umn class: Standard  
polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: C  
Start T: 160 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Da  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromat

360, 1986, 63-78.)NIST Spectranist ri

1777 (Program type: Isothermal; Col... (show more)umn class: Standard  
polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: C  
Start T: 180 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Da  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromat  
360, 1986, 63-78.)NIST Spectranist ri

2739 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capilla  
T: 180 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data ty  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitroben  
3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chro  
356, 1986, 285-299.)NIST Spectranist ri

2764 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capilla  
T: 200 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data ty  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitroben  
3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chro  
356, 1986, 285-299.)NIST Spectranist ri

2781 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0.32 mm; Column length: 25 m; Column type: Capilla  
T: 220 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data ty  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitroben  
3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chro  
356, 1986, 285-299.)NIST Spectranist ri

2753 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0.22 mm; Column length: 25 m; Column type: Capilla  
T: 180 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data ty  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromat  
360, 1986, 63-78.)NIST Spectranist ri

2774 (Program type: Isothermal; Col... (show more)umn class: Standard  
Column diameter: 0.22 mm; Column length: 25 m; Column type: Capilla  
T: 200 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data ty  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analy  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromat  
360, 1986, 63-78.)NIST Spectranist ri

2792 (Program type: Isothermal; Col... (show more)umn class: Standard

Column diameter: 0.22 mm; Column length: 25 m; Column type: Capillary  
T: 220 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data type:  
Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses,  
XLVII. Retention Increments of Some Lower Saturated Branched-Chain,  
Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic and 3, 5-  
Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr.,  
360, 1986, 63-78.)NIST Spectra

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

1761.4 (Program type: Ramp; Column class: Standard non-polar  
Column diameter: 0.33 mm; Column length: 25 m; Column type: Capillary  
rate: 6 K/min; Start T: 100 C; CAS no: 618713; Active phase: SE-30; Carrier  
N2; Data type: Normal alkane RI; Authors: Korhonen, I. O. O., Gas-Liquid  
Chromatographic Analyses. XLVI. Separation of C3-C5 Branched-Chain,  
Unsaturated and Ethyl and .omega.-Chloroethyl Esters of Benzoic, 4-Nitro  
and 3, 5-Dinitrobenzoic acids on SE-30 and OV-351 Capillary Columns with  
Temperature Programming, J. Chromatogr., 357, 1986, 107-118.)NIST Sp  
ri

1761 (Program type: Ramp; Column class: Standard non-polar  
Column diameter: 0.22 mm; Column length: 25 m; Column type: Capillary  
rate: 6 K/min; Start T: 100 C; CAS no: 618713; Active phase: SE-30; Carrier  
N2; Data type: Normal alkane RI; Authors: Korhonen, I. O. O., Gas-Liquid  
Chromatographic Analyses. XLVII. Retention Increments of Some Lower Saturated  
Branched-Chain, Unsaturated and Chlorinated Esters of Benzoic, 4-Nitrobenzoic  
and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J.

Chromatogr., 360, 1986, 63-78.)NIST Spectranist ri

1752 (Program type: Ramp; Column cl... (show more)ass: Semi-standard polar; Column type: Capillary; CAS no: 618713; Active phase: Squalane; type: Normal alkane RI; Authors: Chen, H.-F., Quantitative prediction of gas chromatography retention indices with support vector machines, radial basis neural networks and multiple linear regression, Anal. Chim. Acta, 609, 2008, 36.)NIST Spectranist ri

- **Retention Index (Linear):**

1755 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.33 mm; Column length: 25 m; Column type: Capillary; Flow rate: 6 K/min; Start T: 100 C; End T: 310 C; CAS no: 618713; Active phase: Squalane; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-30 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri

1833 (Program type: Complex; Column... (show more)class: Semi-standard polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Description: Multi-step temperature program; T(initial)= 60C; T(final)= 200C; CAS no: 618713; Active phase: VF-5MS; Carrier gas: He; Phase thickness: 0.25 μm; Data type: Linear RI; Authors: Tretyakov, K. V., Retention Data. NIST Mass Spectrometry Data Center., 2011.)NIST Spectranist ri

2753 (Program type: Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0.32 mm; Column length: 25 m; Column type: Capillary; Heat

K/min; Start T: 100 C; End T: 220 C; CAS no: 618713; Active phase: OV-3  
Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liq  
Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl E  
Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-3  
Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist  
2749 (Program type: Ramp; Column cl... (show more)ass: Standard polar  
diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Heat  
K/min; Start T: 100 C; End T: 220 C; CAS no: 618713; Active phase: OV-3  
Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liq  
Chromatographic Analyses. XLVII. Retention Increments of Some Lower S  
Branched-Chain, Unsaturated and Chlorinated Esters of Benzoic, 4-Nitro  
and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J.  
Chromatogr., 360, 1986, 63-78.)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:	367. 1±22. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 8 mmHg at 25°C
Enthalpy of Vaporization:	61. 4±3. 0 kJ/mol
Flash Point:	171. 8±24. 3 °C
Index of Refraction:	1. 580

Molar Refractivity:	55. 8±0. 3 cm <sup>3</sup>
#H bond acceptors:	8
#H bond donors:	0
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	1. 91
ACD/LogD (pH 5. 5):	2. 05
ACD/BCF (pH 5. 5):	21. 13
ACD/KOC (pH 5. 5):	308. 99
ACD/LogD (pH 7. 4):	2. 05
ACD/BCF (pH 7. 4):	21. 13
ACD/KOC (pH 7. 4):	308. 99
Polar Surface Area:	118 Å <sup>2</sup>
Polarizability:	22. 1±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	58. 3±3. 0 dyne/cm

Molar Volume: 167.5 ± 3.0 cm<sup>3</sup>

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

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 1.95  
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):  
Boiling Pt (deg C): 358.84 (Adapted Stein & Brown method) Melting Pt (deg C): 124.39 (Mean or Weighted MP)  
VP (mm Hg, 25 deg C): 1.75E-005 (Modified Grain method) MP (exp database): 94 deg C  
Subcooled liquid VP: 8.14E-005 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): 233.7 log Kow used: 1.95 (estimated) no-melting pt equation used  
Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 289.44 mg/LECOSAR Class Program (ECOSAR v0. 99h):  
Class(es) found: Dinitrobenzenes Esters Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]:  
Bond Method: 7.17E-010 atm-m<sup>3</sup>/mole Group Method: 1.69E-009 atm-m<sup>3</sup>/mole Henrys LC [VP/WSol estimate using EPI values]: 2.366E-008 atm-m<sup>3</sup>/mole  
Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1.95 (KowWin est)  
Log Kaw used: -7.533 (HenryWin est) Log Koa (KOAWIN v1. 10 estimate): 9.483 Log Koa (experimental database):  
None Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model): 0.1973  
Biowin2 (Non-Linear Model): 0.2076 Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2.4694 (weeks-months)  
Biowin4 (Primary Survey Model): 3.5134 (days-weeks) MITI Biodegradation Probability: Biowin5 (MITI Linear Model): 0.0407  
Biowin6 (MITI Non-Linear Model): 0.0026 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0.2399  
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): 0.0109 Pa (8.14E-005 mm Hg)  
Log Koa (Koawin est): 9.483 Kp (particle/gas partition coef. (m<sup>3</sup>/ug)): Mackay model: 0.000276 Octanol/air (Koa) model: 0.000746  
Fraction sorbed to airborne particulates (phi): Junge-Pankow model: 0.00989 Mackay model: 0.0216 Octanol/air (Koa) model: 0.0564  
Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1.6650 E-12 cm<sup>3</sup>/molecule-sec  
Half-Life = 6.424 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>) Half-Life = 77.086 Hrs Ozone Reaction: No Ozone Reaction Estimation  
Fraction sorbed to airborne particulates (phi): 0.0158 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation  
Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc: 190.2 Log Koc: 2.279 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]:  
Total Kb for pH > 8 at 25 deg C: 4.842E+001 L/mol-sec Kb Half-Life at pH 8: 3.976 hours Kb Half-Life at pH 7: 1.657 days  
Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0.805 (BCF = 6.384)  
log Kow used: 1.95 (estimated) Volatilization from Water: Henry LC: 1.69E-009 atm-m<sup>3</sup>/mole (estimated by Group SAR Method)  
Half-Life from Model River: 5.369E+005 hours (2.237E+004 days) Half-Life from Model Lake: 5.857E+006 hours (2.44E+005 days)  
Removal In Wastewater Treatment: Total removal: 2.20 percent Total biodegradation: 0.10 percent Total sludge adsorption: 2.11 percent  
Total 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. 0165 154 1000 Water 24 900 1000 Soil 75. 9 1. 8e+003 1000  
Sediment 0. 0875 8. 1e+003 0 Persistence Time: 1. 39e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop