

# [Ethyl 3,5-dinitrobenzoate c9h8n2o6 structure](https://assignbuster.com/ethyl-35-dinitrobenzoate-c9h8n2o6-structure/)

Contents

* Retention Index (Linear):

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| --- | --- |
| Molecular Formula  | C 9 H 8 N 2 O 6  |
| Average mass  | 240. 170 Da  |
| Density  | 1. 4±0. 1 g/cm 3  |
| Boiling Point  | 367. 1±22. 0 °C at 760 mmHg  |
| Flash Point  | 171. 8±24. 3 °C  |
| Molar Refractivity  | 55. 8±0. 3 cm 3  |
| Polarizability  | 22. 1±0. 5 10 -24 cm 3  |
| Surface Tension  | 58. 3±3. 0 dyne/cm  |
| Molar Volume  | 167. 5±3. 0 cm 3  |

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

## Experimental Melting Point:

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| --- |
| 91-92 °CAlfa Aesar  |
| 94 °CJean-Claude Bradley Open Melting Point Dataset23389  |
| 92 °CJean-Claude Bradley Open Melting Point Dataset7078  |
| 91-92 °CAlfa AesarB21582  |
| 94-95 °CIndofine[CS-532]  |

* Miscellaneous

## Safety:

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| CAUTION: May irritate eyes, skin, and respiratory tractAlfa AesarB21582  |

* Gas Chromatography

## Retention Index (Kovats):

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| 1951 (estimated with error: 89)NIST Spectramainlib\_117877, replib\_192949, replib\_375615  |
| 1757 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 33 mm; Column length: 25 m; Column type: Capillary; Start T: 160 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 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; Col… (show more)umn class: Standard non-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 type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 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; Col… (show more)umn class: Standard non-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 type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 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; Col… (show more)umn class: Standard non-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 type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 1810 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 33 mm; Column length: 25 m; Column type: Capillary; Start T: 240 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 1752 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 140 C; CAS no: 618713; Active phase: SE-30; 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 Spectranist ri  |
| 1762 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 160 C; CAS no: 618713; Active phase: SE-30; 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 Spectranist ri  |
| 1777 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 180 C; CAS no: 618713; Active phase: SE-30; 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 Spectranist ri  |
| 2739 (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: 618713; Active phase: OV-351; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 2764 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Start T: 200 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 2781 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Start 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. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 2753 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 180 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 Spectranist ri  |
| 2774 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 200 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 Spectranist ri  |
| 2792 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start 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 Spectranist ri  |

## Retention Index (Normal Alkane):

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| 1761. 4 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 33 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data type: Normal alkane RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLVI. Separation of C3-C5 Branched-Chain, C3-C6 Unsaturated and Ethyl and . omega.-Chloroethyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic acids on SE-30 and OV-351 Capillary Columns with Temperature Programming, J. Chromatogr., 357, 1986, 107-118.)NIST Spectranist ri  |
| 1761 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; CAS no: 618713; Active phase: SE-30; Carrier gas: 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 non-polar; Column type: Capillary; CAS no: 618713; Active phase: Squalane; Data type: Normal alkane RI; Authors: Chen, H.-F., Quantitative prediction of gas chromatography retention indices with support vector machines, radial basis neutral networks and multiple linear regression, Anal. Chim. Acta, 609, 2008, 24-36.)NIST Spectranist ri  |

## Retention Index (Linear):

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| --- |
| 1755 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 33 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 310 C; CAS no: 618713; Active phase: SE-30; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 1833 (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: 618713; Active phase: VF-5MS; Carrier gas: He; Phase thickness: 0. 25 um; 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 rate: 6 K/min; Start T: 100 C; End T: 220 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XLV. Retention Behaviour of C1-C12 n-Alkyl Esters of Benzoic, 4-Nitrobenzoic and 3, 5-Dinitrobenzoic Acids on SE-30 and OV-351 Capillary Columns, J. Chromatogr., 356, 1986, 285-299.)NIST Spectranist ri  |
| 2749 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 220 C; CAS no: 618713; Active phase: OV-351; Carrier gas: N2; Data type: Linear 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  |

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

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| Density:  | 1. 4±0. 1 g/cm 3  |
| 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 3  |
| #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 2  |
| Polarizability:  | 22. 1±0. 5 10 -24 cm 3  |
| Surface Tension:  | 58. 3±3. 0 dyne/cm  |
| Molar Volume:  | 167. 5±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. 95Boiling 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 CSubcooled 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. 7log Kow used: 1. 95 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 289. 44 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: DinitrobenzenesEstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 17E-010 atm-m3/moleGroup Method: 1. 69E-009 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 366E-008 atm-m3/moleLog 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. 483Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 1973Biowin2 (Non-Linear Model) : 0. 2076Expert 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. 0407Biowin6 (MITI Non-Linear Model): 0. 0026Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2399Ready 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. 0109 Pa (8. 14E-005 mm Hg)Log Koa (Koawin est ): 9. 483Kp (particle/gas partition coef. (m3/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 cm3/molecule-secHalf-Life = 6. 424 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 77. 086 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0158 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 190. 2Log 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-secKb 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-m3/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 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 11 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. 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

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* 1-Click Scaffold Hop