

# [4,4′-methylenedianiline c13h14n2 structure](https://assignbuster.com/44-methylenedianiline-c13h14n2-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula | C 13 H 14 N 2 |
| Average mass | 198. 264 Da |
| Density | 1. 1±0. 1 g/cm 3 |
| Boiling Point | 398. 0±0. 0 °C at 760 mmHg |
| Flash Point | 221. 1±0. 0 °C |
| Molar Refractivity | 64. 0±0. 3 cm 3 |
| Polarizability | 25. 4±0. 5 10 -24 cm 3 |
| Surface Tension | 54. 0±3. 0 dyne/cm |
| Molar Volume | 173. 4±3. 0 cm 3 |

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

## Experimental Melting Point:

|  |
| --- |
| 91 °CTCIM0220 |
| 88-92 °CAlfa Aesar |
| 92. 5 °CJean-Claude Bradley Open Melting Point Dataset20656 |
| 90 °CJean-Claude Bradley Open Melting Point Dataset4400 |
| 88-92 °CAlfa AesarA15645 |
| 91-94 °CSynQuest72607, 3730-1-07 |
| 91-93 °CLabNetworkLN00225979 |

## Experimental Boiling Point:

|  |
| --- |
| 748 F (397. 7778 °C)NIOSHBY5425000 |
| 232 °C / 9 mm (436. 366 °C / 760 mmHg)Alfa AesarA15645 |
| 257 °C / 18 mmHg (437. 9269 °C / 760 mmHg)SynQuest72607, 3730-1-07 |

## Experimental Ionization Potent:

|  |
| --- |
| 10. 7 EvNIOSHBY5425000 |

## Experimental Flash Point:

|  |
| --- |
| 374 F (190 °C)NIOSHBY5425000 |
| 221 °CAlfa Aesar |
| 221 °F (105 °C)Alfa AesarA15645 |
| 230 °CSynQuest72607, 3730-1-07 |
| 221 °CLabNetworkLN00225979 |

## Experimental Solubility:

|  |
| --- |
| 0. 1%NIOSHBY5425000 |
| -2. 30Egon Willighagenhttp://dx. doi. org/10. 1021/ci050282s |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 91 °CTCI |
| 91 °CTCIM0220 |

* Miscellaneous

## Appearance:

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| Pale-brown, crystalline solid with a faint, amine-like odor. NIOSHBY5425000 |

## Safety:

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| 45-39/23/24/25-43-48/20/21/22-68-51/53Alfa AesarA15645 |
| 53-45-61Alfa AesarA15645 |
| 6. 1Alfa AesarA15645 |
| DangerAlfa AesarA15645 |
| DangerBiosynthW-108903 |
| DANGER: CONTAINS MDA, MAY CAUSE CANCER-LIVER TOXINAlfa AesarA15645 |
| DANGER: POISON, cancer risk, causes liver damageAlfa AesarA15645 |
| GHS07; GHS08; GHS09BiosynthW-108903 |
| H317; H341; H350; H370; H373; H411BiosynthW-108903 |
| H350-H370-H341-H373-H302-H317-H411Alfa AesarA15645 |
| P201; P260; P273; P280; P307+P311BiosynthW-108903 |
| P260-P261-P280-P307+P311-P405-P501aAlfa AesarA15645 |
| R39/23/24/25, R43, R45, R48/20/21/22, R51/53, R68SynQuest3730-1-07, 72607 |
| S22, S24/25, 26, S36/37/39, S45, S53, S61SynQuest3730-1-07, 72607 |
| Toxic/Carcinogenic/Mutagenic/Harmful/Light Sensitive/Air Sensitive/Store under ArgonSynQuest3730-1-07 |

## First-Aid:

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| --- |
| Eye: Irrigate immediately Skin: Soap wash immediately Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHBY5425000 |

## Exposure Routes:

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| --- |
| inhalation, skin absorption, ingestion, skin and/or eye contactNIOSHBY5425000 |

## Symptoms:

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| --- |
| Irritation eyes; jaundice, hepatitis; myocardial damage; in animals: heart, liver, spleen damage; [potential occupational carcinogen]NIOSHBY5425000 |

## Target Organs:

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| --- |
| Eyes, liver, cardiovascular system, spleen Cancer Site [in animals: bladder cancer]NIOSHBY5425000 |

## Incompatibility:

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| --- |
| Strong oxidizersNIOSHBY5425000 |

## Personal Protection:

|  |
| --- |
| Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated/Daily Remove: When wet or contaminated Change: Daily Provide: Eyewash, Quick drenchNIOSHBY5425000 |

## Exposure Limits:

|  |
| --- |
| NIOSH REL : Ca See Appendix A OSHA PEL : [1910. 1050] TWA 0. 010 ppm ST 0. 100 ppmNIOSHBY5425000 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 2090 (estimated with error: 83)NIST Spectramainlib\_228923, replib\_220964, replib\_291143 |

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

|  |  |
| --- | --- |
| Density: | 1. 1±0. 1 g/cm 3 |
| Boiling Point: | 398. 0±0. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 9 mmHg at 25°C |
| Enthalpy of Vaporization: | 64. 9±3. 0 kJ/mol |
| Flash Point: | 221. 1±0. 0 °C |
| Index of Refraction: | 1. 660 |
| Molar Refractivity: | 64. 0±0. 3 cm 3 |
| #H bond acceptors: | 2 |
| #H bond donors: | 4 |
| #Freely Rotating Bonds: | 2 |
| #Rule of 5 Violations: | 0 |

|  |  |
| --- | --- |
| ACD/LogP: | 1. 64 |
| ACD/LogD (pH 5. 5): | 1. 45 |
| ACD/BCF (pH 5. 5): | 6. 57 |
| ACD/KOC (pH 5. 5): | 115. 37 |
| ACD/LogD (pH 7. 4): | 1. 68 |
| ACD/BCF (pH 7. 4): | 11. 04 |
| ACD/KOC (pH 7. 4): | 193. 71 |
| Polar Surface Area: | 52 Å 2 |
| Polarizability: | 25. 4±0. 5 10 -24 cm 3 |
| Surface Tension: | 54. 0±3. 0 dyne/cm |
| Molar Volume: | 173. 4±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. 18Log Kow (Exper. database match) = 1. 59Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 367. 40 (Adapted Stein & Brown method)Melting Pt (deg C): 127. 52 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 07E-006 (Modified Grain method)MP (exp database): 92. 5 deg CBP (exp database): 398 deg CSubcooled liquid VP: 9. 3E-006 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): 1959log Kow used: 1. 59 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 1000 mg/L (25 deg C)Exper. Ref: MOORE, WM (1978)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 82. 535 mg/LWat Sol (Exper. database match) = 1000. 00Exper. Ref: MOORE, WM (1978)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 99E-011 atm-m3/moleGroup Method: 1. 58E-011 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 757E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 59 (exp database)Log Kaw used: -8. 611 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 10. 201Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2403Biowin2 (Non-Linear Model) : 0. 0455Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 4163 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2764 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 1830Biowin6 (MITI Non-Linear Model): 0. 0080Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 6048Ready 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. 00124 Pa (9. 3E-006 mm Hg)Log Koa (Koawin est ): 10. 201Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00242 Octanol/air (Koa) model: 0. 0039 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0804 Mackay model : 0. 162 Octanol/air (Koa) model: 0. 238 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 200. 9340 E-12 cm3/molecule-secHalf-Life = 0. 053 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 639 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 121 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 4950Log Koc: 3. 695 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. 524 (BCF = 3. 344)log Kow used: 1. 59 (expkow database)Volatilization from Water: Henry LC: 1. 58E-011 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 5. 218E+007 hours (2. 174E+006 days)Half-Life from Model Lake : 5. 692E+008 hours (2. 372E+007 days)Removal In Wastewater Treatment: Total removal: 2. 00 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 91 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. 000183 8. 56 1000 Water 31. 1 900 1000 Soil 68. 8 1. 8e+003 1000 Sediment 0. 0831 8. 1e+003 0 Persistence Time: 1. 23e+003 hr

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