4,4′-methylenedianiline c13h14n2 structure

Contents

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:

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

NIOSHBY5425000

Safety:

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 AesarA1

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,

S22, S24/25, 26, S36/37/39, S45, S53, S61SynQuest3730-1-07, 72607

Toxic/Carcinogenic/Mutagenic/Harmful/Light Sensitive/Air Sensitive/Store

ArgonSynQuest3730-1-07

- **First-Aid:**

  Eye: Irrigate immediately Skin: Soap wash immediately Breathing: Respi

  support Swallow: Medical attention immediatelyNIOSHBY5425000

- **Exposure Routes:**

  inhalation, skin absorption, ingestion, skin and/or eye

  contactNIOSHBY5425000

- **Symptoms:**

  Irritation eyes; jaundice, hepatitis; myocardial damage; in animals: heart

  spleen damage; [potential occupational carcinogen]NIOSHBY5425000

- **Target Organs:**

  Eyes, liver, cardiovascular system, spleen Cancer Site [in animals: bladde

  cancer]NIOSHBY5425000

- **Incompatibility:**

  Strong

oxidizersNIOSHBY5425000

- **Personal Protection:**

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

- **Exposure Limits:**

  NIOSH REL : Ca See Appendix A OSHA PEL : [1910. 1050] TWA 0. 010 ppr 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

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop