4-chloro-o-toluidine c7h8cln structure

Contents

- Retention Index (Linear):

Molecular Formula	C_7H_8ClN
Average mass	141. 598 Da
Density	1. 2±0. 1 g/cm ^{3}
Boiling Point	242. 8±20. 0 °C at 760 mmHg
Flash Point	99. 4±0. 0 °C
Molar Refractivity	40. 2±0. 3 cm ^{3}
Polarizability	15. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	42. 7±3. 0 dyne/cm
Molar Volume	119. 9±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs

- Predicted – EPISuite
- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties
    - **Experimental Melting Point:**

      24-27

      °COakwood[02487

      2]

      30. 3 °CJean-

      Claude Bradley

      Open Melting Point

      Dataset20828

      24-27 °CMatrix

      Scientific

      24-27 °CMatrix

      Scientific074482

      24-30

      °CSynQuest74241,

      3630-5-Z5

      24-27

      °COakwood[02487

2]

- **Experimental Boiling Point:**

  241 °COakwood[024872]

  241 °CMatrix Scientific

  241 °CMatrix

  Scientific074482

  241 °CSynQuest74241,

  3630-5-Z5

  241 °COakwood[024872]

- **Experimental LogP:**

  2. 216Vitas-

  MSTL163571

- **Experimental Flash Point:**

  25 °CTCIA0704

  124 °CSynQuest74241,

  3630-5-Z5

  124 °COakwood[024872]

- **Experimental Gravity:**

  1. 19 g/mLSynQuest3630-

  5-Z5

  1. 14

  g/mLOakwood[024872]

- **Experimental Refraction Index:**

  1. 58SynQuest74241,

  3630-5-Z5

- Miscellaneous

- **Appearance:**

  Not

  AvailableNovochem

  y[NC-30682]

- **Safety:**

  20/21/22Novochem

  y[NC-30682]

  20/21/36/37/39Nov

  ochemy[NC-30682]

  GHS07;

  GHS09Novochemy[

NC-30682]

H332;
H403Novochemy[N
C-30682]

P332+P313;
P305+P351+P338N
ovochemy[NC-
30682]

R52/53Novochemy[
NC-30682]

TOXICMatrix
Scientific074482

Toxic/
Carcinogenic/
Mutagenic/Light
Sensitive/Keep
ColdSynQuest3630-
5-Z5, 74241

WarningNovochem
y[NC-30682]

- Gas Chromatography

- **Retention Index (Kovats):**

  1285 (estimated with error: 89)NIST Spectramainlib_230019, replib_69505, replib_221225

- **Retention Index (Linear):**

  1247. 3 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 325 C; CAS no: 95692; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors:

Sun, G.; Stremple, P., Retention index characterization of flavor, fragrance, and many other compounds on DB-1 and DB-XLB, 2003.)NIST Spectranist ri

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

Density:	1. 2±0. 1 g/cm ^{3}
Boiling Point:	242. 8±20. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	48. 0±3. 0 kJ/mol
Flash Point:	99. 4±0. 0 °C
Index of Refraction:	1. 585
Molar Refractivity:	40. 2±0. 3 cm ^{3}
#H bond acceptors:	1
#H bond donors:	2

#Freely Rotating Bonds:	0
#Rule of 5 Violations:	0
ACD/LogP:	2. 22
ACD/LogD (pH 5. 5):	2. 01
ACD/BCF (pH 5. 5):	19. 67
ACD/KOC (pH 5. 5):	291. 94
ACD/LogD (pH 7. 4):	2. 02
ACD/BCF (pH 7. 4):	20. 08
ACD/KOC (pH 7. 4):	297. 86
Polar Surface Area:	26 Å ^{2}
Polarizability:	15. 9±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	42. 7±3. 0 dyne/cm
Molar Volume:	119. 9±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. 27Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 234. 76 (Adapted Stein & Brown method)Melting Pt (deg C): 41. 77 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0324 (Modified Grain method)MP (exp database): 30. 3 deg CBP (exp database): 244 deg CSubcooled liquid VP: 0. 0362 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): 953. 9log Kow used: 2. 27 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1732. 4 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 56E-006 atm-m3/moleGroup Method: 1. 99E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 6. 328E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 27 (KowWin est)Log Kaw used: -4. 195 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 465Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3186Biowin2 (Non-Linear Model) : 0. 0873Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 4699 (weeks-months)Biowin4 (Primary Survey Model) : 3. 3012 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2055Biowin6 (MITI Non-Linear Model): 0. 0879Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 5021Ready 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): 4. 83 Pa (0. 0362 mm Hg)Log Koa (Koawin est): 6. 465Kp (particle/gas partition coef. (m3/ug)): Mackay model : 6. 22E-007 Octanol/air (Koa) model: 7. 16E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 24E-005 Mackay model : 4. 97E-005 Octanol/air (Koa) model: 5. 73E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 38. 6643 E-12 cm3/molecule-secHalf-Life = 0. 277 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 320 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 3. 61E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 119. 9Log Koc: 2. 079 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 = 1. 046 (BCF = 11. 12)log Kow used: 2. 27 (estimated)Volatilization from Water: Henry LC: 1. 99E-006 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 351. 3 hours (14. 64 days)Half-Life from Model Lake : 3932 hours (163. 8 days)Removal In Wastewater Treatment: Total removal: 2. 70 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 49 percentTotal to Air: 0. 11 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 351 6. 64 1000 Water 26. 3 900 1000 Soil 73. 2 1. 8e+003 1000 Sediment 0. 146 8. 1e+003 0 Persistence Time: 871 hrLog Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 27Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 234. 76 (Adapted Stein & Brown method)Melting Pt (deg C): 41. 77 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0324 (Modified Grain method)MP (exp database): 30. 3 deg CBP (exp database): 244 deg CSubcooled liquid VP: 0. 0362 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): 953. 9log Kow used: 2. 27 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1732. 4 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 56E-006 atm-m3/moleGroup Method: 1. 99E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]:

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- 1-Click Scaffold Hop