

# [4-chloro-o-toluidine c7h8cln structure](https://assignbuster.com/4-chloro-o-toluidine-c7h8cln-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 7 H 8 ClN |
| 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[024872] |
| 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[024872] |

## 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 AvailableNovochemy[NC-30682] |

## Safety:

|  |
| --- |
| 20/21/22Novochemy[NC-30682] |
| 20/21/36/37/39Novochemy[NC-30682] |
| GHS07; GHS09Novochemy[NC-30682] |
| H332; H403Novochemy[NC-30682] |
| P332+P313; P305+P351+P338Novochemy[NC-30682] |
| R52/53Novochemy[NC-30682] |
| TOXICMatrix Scientific074482 |
| Toxic/Carcinogenic/Mutagenic/Light Sensitive/Keep ColdSynQuest3630-5-Z5, 74241 |
| WarningNovochemy[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! 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