

# [Pentacontane c50h102 structure](https://assignbuster.com/pentacontane-c50h102-structure/)

Contents

* Predicted Melting Point:

|  |  |
| --- | --- |
| Molecular Formula  | C 50 H 102  |
| Average mass  | 703. 345 Da  |
| Density  | 0. 8±0. 1 g/cm 3  |
| Boiling Point  | 578. 4±13. 0 °C at 760 mmHg  |
| Flash Point  | 507. 6±9. 4 °C  |
| Molar Refractivity  | 233. 7±0. 3 cm 3  |
| Polarizability  | 92. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 31. 4±3. 0 dyne/cm  |
| Molar Volume  | 853. 9±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 94 °CTCIP0964  |
| 94 °CIndofine[05-5000],[05-5000]  |
| 94 °CIndofine[05-5000],[05-5000],[05-5000]  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 94 °CTCI  |
| 94 °CTCIP0964  |

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

|  |  |
| --- | --- |
| Density:  | 0. 8±0. 1 g/cm 3  |
| Boiling Point:  | 578. 4±13. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 8 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 83. 4±0. 8 kJ/mol  |
| Flash Point:  | 507. 6±9. 4 °C  |
| Index of Refraction:  | 1. 460  |
| Molar Refractivity:  | 233. 7±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 47  |
| #Rule of 5 Violations:  | 2  |

|  |  |
| --- | --- |
| ACD/LogP:  | 27. 32  |
| ACD/LogD (pH 5. 5):  | 24. 85  |
| ACD/BCF (pH 5. 5):  | 1000000. 00  |
| ACD/KOC (pH 5. 5):  | 10000000. 00  |
| ACD/LogD (pH 7. 4):  | 24. 85  |
| ACD/BCF (pH 7. 4):  | 1000000. 00  |
| ACD/KOC (pH 7. 4):  | 10000000. 00  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 92. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 31. 4±3. 0 dyne/cm  |
| Molar Volume:  | 853. 9±3. 0 cm 3  |

Click to predict properties on the Chemicalize site