

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

Contents

* Predicted Melting Point:

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| --- | --- |
| 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

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| --- | --- |
| 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 |

|  |  |
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| 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