

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
 $^{\circ}C$ at 760
mmHg

Flash Point $507.6 \pm 9.$
 $4^{\circ}C$

Molar $233.7 \pm 0.$

Refractivity $3 cm^3$

Polarizabilit
y 92.6 ± 0.5
 $10^{-24} cm^3$

Surface 31.4 ± 3.0

Tension dyne/cm

Molar 853. 9±3.

Volume 0 cm³

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

- **Experimental Melting Point:**

94

°CTCIP096

4

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