

1,8-  
diiodoperfluorooctane  
c8f16i2 structure



**ASSIGN  
BUSTER**

## Contents

- Safety:

Molecular Formula	$C_8F_{16}I_2$
Average mass	653.869 Da
Density	$2.3 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$222.0 \pm 8.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$98.5 \pm 5.6 \text{ }^\circ\text{C}$
Molar Refractivity	$67.4 \pm 0.3 \text{ cm}^3$
Polarizability	$26.7 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$20.9 \pm 3.0$ dyne/cm
Molar Volume	$285.8 \pm 3.0$ $\text{cm}^3$

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

- **Experimental Melting Point:**

75-76

°CSynQuest

75-76

°CSynQuest9152

, 1100-J-19

- **Experimental Boiling Point:**

112 °C / 25

mmHg (235.

6772 °C / 760

mmHg)SynQuest

9152, 1100-J-19

- **Experimental Flash Point:**

- Miscellaneous

- **Safety:**

Irritant/Keep

ColdSynQuest11

00-J-19, 9152

R36/37/38SynQu

est1100-J-19,

9152

S3, S15, S22,

S24/25, S26,

S36/37/39,

S45SynQuest11

00-J-19

S3, S15, S22,

S24/25,

S36/37/39,

S45SynQuest11

00-J-19, 9152

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

Density:  $2.3 \pm 0.1 \text{ g/cm}^3$

Boiling Point:  $222.0 \pm 8.0 \text{ }^\circ\text{C}$  at 760 mmHg

Vapour Pressure:  $0.2 \pm 0.4 \text{ mmHg}$  at  $25^\circ\text{C}$

Enthalpy of Vaporization:  $44.0 \pm 3.0 \text{ kJ/mol}$

Flash Point:	98.5 ± 5.6 °C
Index of Refraction:	1.388
Molar Refractivity:	67.4 ± 0.3 cm <sup>3</sup>
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	7
#Rule of 5 Violations:	2
ACD/LogP:	10.56
ACD/LogD (pH 5.5):	8.41
ACD/BCF (pH 5.5):	1000000.00
ACD/KOC (pH 5.5):	893926.00
ACD/LogD (pH 7.4):	8.41
ACD/BCF (pH 7.4):	1000000.00
ACD/KOC (pH 7.4):	893926.00
Polar Surface Area:	0 Å <sup>2</sup>
Polarizability:	26.7 ± 0.5 10 <sup>-24</sup> cm <sup>3</sup>

Surface Tension:  $20.9 \pm 3.0$  dyne/cm

Molar Volume:  $285.8 \pm 3.0$  cm<sup>3</sup>

Click to predict properties on the Chemicalize site