4-fluorophenethylamine c8h10fn structure

Contents

- Retention Index (Kovats):

Molecular Formula	$C_8H_{10}FN$
Average mass	139. 170 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	251. 7±0. 0 °C at 760 mmHg
Flash Point	78. 9±0. 0 °C
Molar Refractivity	39. 3±0. 3 cm ^{3}
Polarizability	15. 6±0. 5 10^{-24} cm ^{3}
Surface Tension	36. 6±3. 0 dyne/cm
Molar Volume	130. 1±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Boiling Point:

50-52 deg C / 0. 1

mmHg (317. 8095-321.

3192 °C / 760

mmHg)Manchester

OrganicsA18022

50-52 °CMatrix

Scientific

50-52 °CAlfa

AesarH61791

50-52 °CMatrix

Scientific075296

50-52 °C / 0. 15 mmHg

(306. 135-309. 5784 °C

/ 760

mmHg)SynQuest51873

, 3630-3-X1

Experimental LogP:

1. 51Vitas-

MSTL163864

- **Experimental Flash Point:**

  79 °CAlfa Aesar

  79 °F (26. 1111 °C)Alfa AesarH61791

  79 °CSynQuest51873, 3630-3-X1

  79 °CLabNetworkLN00009057

- **Experimental Gravity:**

  25 g/mLSynQuest3630-3-X1

  1. 061 g/mLAlfa AesarH61791

  1. 061 g/mLMatrix Scientific075296

  1. 061 g/mLSynQuest3630-3-X1

- **Experimental Refraction Index:**

  1. 5072SynQuest51873, 3630-3-X1

- Miscellaneous

- **Appearance:**

  Yellow liquidNovochemy[NC-29974]

- **Safety:**

  20/21/36/37/39Novochemy[NC-29974]

  23/24/25-34Alfa AesarH61791

  36/37/38Novochemy[NC-29974]

  4-9-20-23-26-27-36/37/39-45-60Alfa AesarH61791

  8Alfa AesarH61791

  DangerAlfa AesarH61791

  DangerBiosynthW-107996

GHS02; GHS07;

GHS09Novochemy[NC-

29974]

GHS05;

GHS06BiosynthW-

107996

H301; H311; H314;

H331BiosynthW-

107996

H301-H311-H330-

H314Alfa AesarH61791

H332;

H403Novochemy[NC-

29974]

IRRITANTMatrix

Scientific075296

P102; P210; P262;

P270; P302+P352;

P308+P313Novochemy

[NC-29974]

P260-P301+P310-

P303+P361+P353-

P304+P340-

P305+P351+P338-

P320-P330-P361-P405-

P501aAlfa

AesarH61791

P261; P280;

P305+P351+P338;

P310BiosynthW-

107996

R52/53Novochemy[NC-

29974]

WarningNovochemy[NC

-29974]

- Gas Chromatography

- **Retention Index (Kovats):**

  1111 (estimated with

  error: 89)NIST

  Spectramainlib_237858

  , replib_108036

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

Density:	1. 1±0. 1 g/cm ^{3}

Boiling Point:	251. 7±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	48. 9±3. 0 kJ/mol
Flash Point:	78. 9±0. 0 °C
Index of Refraction:	1. 516
Molar Refractivity:	39. 3±0. 3 cm^3
#H bond acceptors:	1
#H bond donors:	2
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	1. 51
ACD/LogD (pH 5. 5):	-1. 57
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-0. 85
ACD/BCF (pH 7. 4):	1. 00

ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	26 Å ^{2}
Polarizability:	15. 6±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	36. 6±3. 0 dyne/cm
Molar Volume:	130. 1±3. 0 cm ^{3}

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

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