

# [4-fluorophenethylamine c8h10fn structure](https://assignbuster.com/4-fluorophenethylamine-c8h10fn-structure/)

Contents

* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula | C 8 H 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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