

# [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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