

# [Choline chloride c5h14clno structure](https://assignbuster.com/choline-chloride-c5h14clno-structure/)

Contents

* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula | C 5 H 14 ClNO |
| Average mass | 139. 624 Da |
| Density |  |
| Boiling Point |  |
| Flash Point |  |
| Molar Refractivity |  |
| Polarizability |  |
| Surface Tension |  |
| Molar Volume |  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 305 °C (Decomposes)Alfa Aesar |
| 305 °C (Decomposes)Alfa AesarA15828 |
| 303-305 °CJ&K Scientific185888 |
| 302-305 °CIndofine[BIO-108] |
| 302-303 °CFooDBFDB000711 |

## Experimental Solubility:

|  |
| --- |
| 500 mg/ml in H2O, 28 mg/ml in DMSO (at 25°C)MedChem Expresshttp://www. medchemexpress. com/Fusidic-acid-sodium-salt. html, HY-B1337 |
| H2O: 1 M, clear, colorlessIndofine[BIO-108] |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 303-305 °CJ&K Scientific185888 |

* Miscellaneous

## Appearance:

|  |
| --- |
| deliquescent crystalsOxford University Chemical Safety Data (No longer updated)More details |

## Stability:

|  |
| --- |
| Stable. Incompatible with strong oxidizing agents, moisture. Store under a dry atmosphere. Oxford University Chemical Safety Data (No longer updated)More details |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 3400 mg kg-1, IPR-MUS LD50 320 mg kg-1, ORL-MUS LD50 3900 mg kg-1, IVN-MUS LD50 53 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details |

## Safety:

|  |
| --- |
| 26-37Alfa AesarA15828 |
| 26-37-60Alfa AesarA15828 |
| 36/37/38Alfa AesarA15828 |
| CAUTION: May irritate eyes, skin, and respiratory tractAlfa AesarA15828 |
| H315-H319-H335Alfa AesarA15828 |
| Minimize contact. Oxford University Chemical Safety Data (No longer updated)More details |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA15828 |
| WarningAlfa AesarA15828 |
| WARNING: Irritates lungs, eyes, skinAlfa AesarA15828 |
| XiAbblis ChemicalsAB1002139 |

## Target Organs:

|  |
| --- |
| AChR agonistTargetMolT1039 |

## Chemical Class:

|  |
| --- |
| alkaloidMicrosource[01503428] |

## Compound Source:

|  |
| --- |
| widespread in the plant and animal kingdomsMicrosource[01503428] |

## Bio Activity:

|  |
| --- |
| Choline chloride is an organic compound and a quaternary ammonium salt, an acyl group acceptor and choline acetyltransferase substrate, also is an important additive in feed especially for chickens where it accelerates growth. MedChem Expresshttp://www. medchemexpress. com/Fusidic-acid-sodium-salt. html |
| Choline chloride is an organic compound and a quaternary ammonium salt, an acyl group acceptor and choline acetyltransferase substrate, also is an important additive in feed especially for chickens where it accelerates growth. MedChem ExpressHY-B1337 |
| Muscarinic AChRTargetMolT1039 |
| NeuroscienceTargetMolT1039 |
| OthersMedChem ExpressHY-B1337 |

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

No predicted properties have been calculated for this compound.

|  |  |
| --- | --- |
| Density: |  |
| Boiling Point: |  |
| Vapour Pressure: |  |
| Enthalpy of Vaporization: |  |
| Flash Point: |  |
| Index of Refraction: |  |
| Molar Refractivity: |  |
| #H bond acceptors: |  |
| #H bond donors: |  |
| #Freely Rotating Bonds: |  |
| #Rule of 5 Violations: |  |

|  |  |
| --- | --- |
| ACD/LogP: |  |
| ACD/LogD (pH 5. 5): |  |
| ACD/BCF (pH 5. 5): |  |
| ACD/KOC (pH 5. 5): |  |
| ACD/LogD (pH 7. 4): |  |
| ACD/BCF (pH 7. 4): |  |
| ACD/KOC (pH 7. 4): |  |
| Polar Surface Area: |  |
| Polarizability: |  |
| Surface Tension: |  |
| Molar Volume: |  |

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop