



# ChemSpider

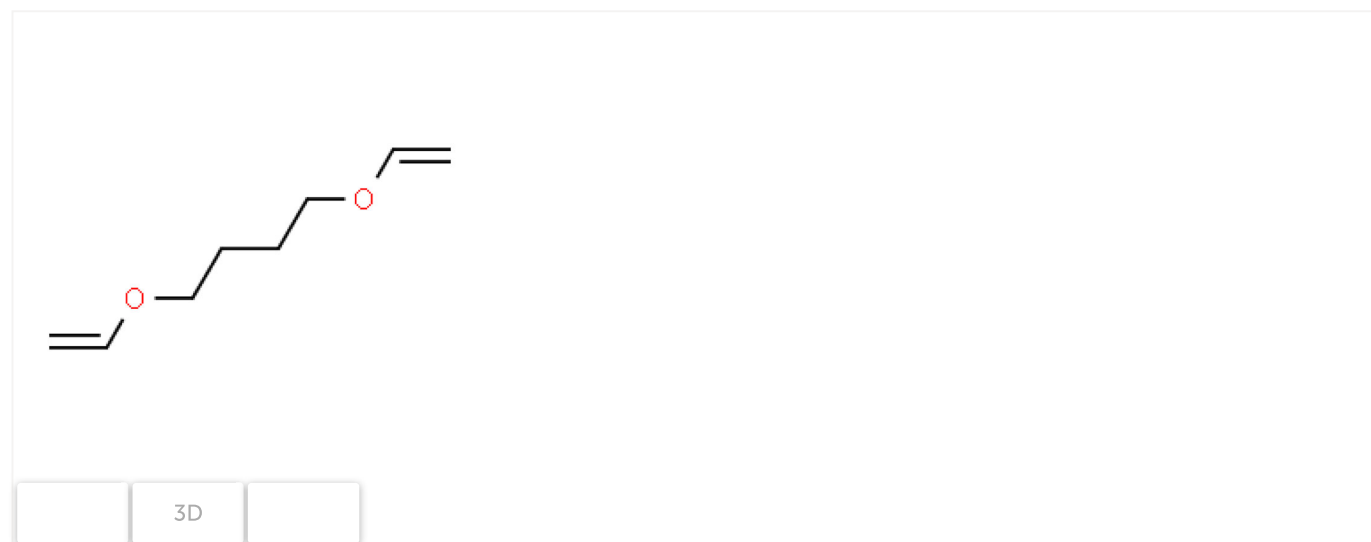
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Search term: **3891-33-6** (Found by approved synonym)



## MFCD00026065

Molecular Formula

C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>

Average mass

142.196 Da

Monoisotopic mass

142.099380 Da

More details:

[Names](#)

[Properties](#)

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- [Experimental data](#)
- [Predicted - ACD/Labs](#)

Feedback





- [Predicted - Mcule](#)

## Experimental Physico-chemical Properties

Experimental Melting Point:

Experimental Boiling Point:

62-64 °C / 10 mmHg **Parchem – fine & specialty chemicals** [71711](#)

62-64 °C / 10 mmHg (199.4595-202.204 °C / 760 mmHg) **Sigma-Aldrich** [ALDRICH-123315](#)

Experimental Flash Point:

Experimental Refraction Index:

Experimental Density:

## Gas Chromatography

Retention Index (Kovats):

948 (estimated with error: 68) **NIST Spectra** [mainlib\\_288954](#)

**Predicted data is generated using the [ACD/Labs Percepta Platform - PhysChem Module](#), version: 14.00**

Feedback

**Density:** 0.9±0.1 g/cm<sup>3</sup>

**Boiling Point:** 191.1±13.0 °C at 760 mmHg

**Vapour Pressure:** 0.7±0.4 mmHg at 25°C

**Enthalpy of Vaporization:** 41.0±3.0 kJ/mol

**Flash Point:** 60.1±19.4 °C

**Index of Refraction:** 1.428

**Molar Refractivity:** 42.1±0.3 cm<sup>3</sup>



|                                     |                                            |
|-------------------------------------|--------------------------------------------|
| #H bond donors:                     | 0                                          |
| #Freely Rotating Bonds:             | 7                                          |
| #Rule of 5 Violations:              | 0                                          |
| <a href="#">ACD/LogP:</a>           | 1.53                                       |
| <a href="#">ACD/LogD (pH 5.5):</a>  | 1.65                                       |
| <a href="#">ACD/BCF (pH 5.5):</a>   | 10.66                                      |
| <a href="#">ACD/KOC (pH 5.5):</a>   | 189.41                                     |
| <a href="#">ACD/LogD (pH 7.4):</a>  | 1.65                                       |
| <a href="#">ACD/BCF (pH 7.4):</a>   | 10.66                                      |
| <a href="#">ACD/KOC (pH 7.4):</a>   | 189.41                                     |
| <a href="#">Polar Surface Area:</a> | 18 Å <sup>2</sup>                          |
| <a href="#">Polarizability:</a>     | 16.7±0.5 10 <sup>-24</sup> cm <sup>3</sup> |
| <a href="#">Surface Tension:</a>    | 25.6±3.0 dyne/cm                           |
| <a href="#">Molar Volume:</a>       | 163.5±3.0 cm <sup>3</sup>                  |

Predicted data is generated using the [US Environmental Protection Agency's EPI Suite™](#)