

# Ethyl (trimethylsilyl)acetate

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Ethyl (2-trimethylsilyl)acetate<br>Acetic acid, (trimethylsilyl)-, ethyl ester |
| <b>Inchi:</b>               | InChI=1S/C7H16O2Si/c1-5-9-7(8)6-10(2,3)4/h5-6H2,1-4H3                          |
| <b>InchiKey:</b>            | QQFBQBDINHJDMN-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C7H16O2Si  |
| <b>SMILES:</b>              | CCOC(=O)C[Si](C)(C)C   |
| <b>Mol. weight [g/mol]:</b> | 160.29   |
| <b>CAS:</b>                 | 4071-88-9  |

## Physical Properties

| Property code | Value         | Unit | Source         |
|---------------|---------------|------|----------------|
| log10ws       | 0.92          |      | Crippen Method |
| logp          | 1.888         |      | Crippen Method |
| rinpol        | 942.00        |      | NIST Webbook   |
| rinpol        | 930.00        |      | NIST Webbook   |
| tb            | 430.00 ± 1.00 | K    | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4071889&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4071889&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |

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