Alkylation Reagents for Ester Synthesis

Methylation Reagents
Methylation Reagents (Diazomethane Precursors/Equivalents)
Ethylation Reagents
Propylation & Isopropylation Reagents
Butylation & tert-Butylation Reagents
Other Alkylation Reagents
Carboxylic acid esters are basic compounds in organic chemistry, and have a wide range of uses as various chemical products such as pharmaceuticals, agrochemicals, cosmetics, flavors, and electronic materials, and their synthetic intermediates.

As for synthetic methods of ester compounds, ‘Fisher esterification’ is well-known since a long time ago, by which ester compounds can be synthesized using carboxylic acids and alcohols in the presence of acid catalysts. This reaction is reversible, and it is possible to obtain the desired esters by using excess amount of alcohols, or removing water under azeotropic condition.

\[
\text{RCOOH} + \text{R'}\text{OH} \underset{\text{Acid, } \Delta}{\overset{\text{Acid, } \Delta}{\rightleftharpoons}} \text{RCOR'} + \text{H}_2\text{O}
\]

As other traditional synthetic method, the methylation reaction of carboxylic acids is also known using in situ generated diazomethane. This reaction proceeds fast under neutral condition. However, since there are several reports on the explosive and cancer-causing property of diazomethane, trimethylsilyldiazomethane – hexane solution (T1146), which is less explosive, has been used as an alternative to diazomethane in recent years.

In addition to these reactions above, various kinds of synthetic methods for ester synthesis by alkylation carboxylic acids have been also reported as below.

1. Alkylation of Carboxylic Acids using Orthoesters

2. Alkylation of Carboxylic Acids using \(N,N\)-Dimethylformamide Dialkyl Acetals

3. Alkylation of Carboxylic Acids using Triazene Derivatives

4. Alkylation of Carboxylic Acids using \(O\)-Dialkylisoureas

TCI offers a variety of alkylation reagents for ester synthesis other than the reagents above. All the products are listed as below.

References

1. E. Fischer, A. Speer, Ber. 1895, 28, 3252.
### Methylation Reagents

**X0036** 1set
Boron Trifluoride - Methanol Reagent (10-20%)
CAS RN: 373-57-9

**O0068** 25mL 500mL
Trimethyl Orthoformate
CAS RN: 149-73-5

**D0271** 25mL
N,N-Dimethylformamide Dimethyl Acetal
CAS RN: 4637-24-5

**D1332** 1set
N,N-Dimethylformamide Dimethyl Acetal (0.5mL×10)
CAS RN: 4637-24-5

**M0641** 1g 25g
1-Methyl-3-p-tolyltetrazene
CAS RN: 21124-13-0

**D4587** 5mL
N,N'-Diisopropyl-O-methylisourea
CAS RN: 54648-79-2

**T0269** 25g 500g
Methyl p-Toluenesulfonate
CAS RN: 80-48-8

**T1576** 5mL 25mL
Trimethylsulfoxonium Hydroxide (0.2mol/L in Methanol)
CAS RN: 17287-03-5

### Methylation Reagents (Diazomethane Precursors & Equivalents)

**T1146** 10mL 25mL 100mL
Trimethylsilidiazomethane
CAS RN: 18107-18-1

**T0323** 25g 500g
N-Methyl-N-nitroso-p-toluenesulfonamide
CAS RN: 80-11-5

**N0265** 5g 25g
N-Methyl-N-nitrosourethane
CAS RN: 615-53-2

**M0527** 5g 25g
1-Methyl-3-nitro-1-nitrosoguanidine (wetted with ca. 50% Water, containing 5g on a dry weight basis)
CAS RN: 70-25-7

### Ethylation Reagents

**O0066** 25mL 500mL
Triethyl Orthoformate
CAS RN: 122-51-0

**D1294** 5mL 25mL
N,N-Dimethylformamide Diethyl Acetal
CAS RN: 1188-33-6

**E0292** 1g
1-Ethyl-3-p-tolytriene
CAS RN: 50707-40-9

Please inquire for pricing and availability of listed products to our local sales representatives.
Alkylation Reagents for Ester Synthesis

### Alkylation Reagents for Ester Synthesis

- **E1058**: 5mL 25mL
  - O-Ethyl-N,N'-diisopropylisourea
  - CAS RN: 60683-30-9
- **B0588**: 25g 500g
  - CH₃CH₂Br
  - Bromoethane
  - CAS RN: 74-96-4
- **I0058**: 25g 100g 500g
  - CH₃CH₂I
  - Iodoethane (stabilized with Copper chip)
  - CAS RN: 75-03-6
- **C0041**: 25g 500g
  - CH₃O⁻CH₂CH₃
  - Diethyl Carbonate
  - CAS RN: 105-58-8
- **D0525**: 25mL 500mL
  - CH₃SO⁻CH₂CH₃
  - Diethyl Sulfate
  - CAS RN: 64-67-5

### Propylation & Isopropylation Reagents

- **M0607**: 25g 100g
  - CH₃(CH₂)₃O⁻CH₂CH₃
  - Ethyl Methanesulfonate
  - CAS RN: 62-50-0
- **T0268**: 25g 500g
  - CH₃CH₂Br
  - Bromoethane
  - CAS RN: 74-96-4

### Butylation & tert-Butylation Reagents

- **X0037**: 1set
  - Boron Trifluoride - Propanol Reagent (10-20%)
  - CAS RN: 762-48-1
- **O0259**: 25mL 500mL
  - OCH₂CH₂CH₃
  - Tripropyl Orthoformate
  - CAS RN: 621-76-1

### Butylation & tert-Butylation Reagents

- **D1302**: 5mL 25mL
  - CH₃(CH₂)₃O⁻CH₂CH₃
  - Tributyl Orthoformate
  - CAS RN: 692-39-7
**Alkylation Reagents for Ester Synthesis**

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<th>Code</th>
<th>Quantity</th>
<th>CAS RN</th>
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<td><strong>Butyl p-Toluenesulfonate</strong></td>
<td>25mL 500mL</td>
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<td><strong>Heptyl p-Toluenesulfonate</strong></td>
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<td>3386-35-4</td>
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