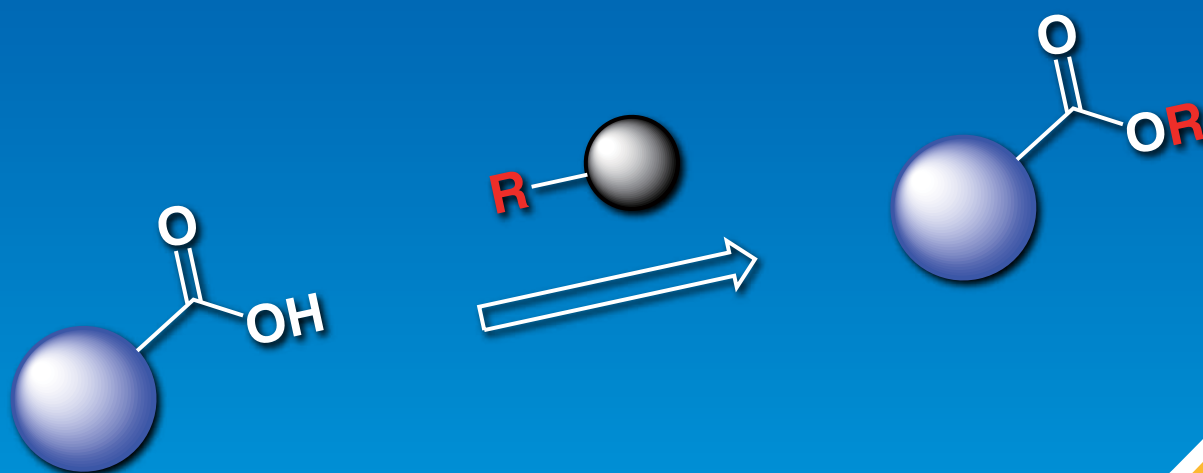


Alkylation Reagents for Ester Synthesis



Methylation Reagents

Methylation Reagents (Diazomethane Precursors/Equivalents)

Ethylation Reagents

Propylation & Isopropylation Reagents

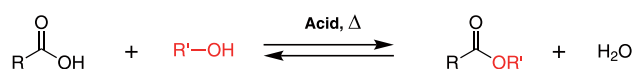
Butylation & *tert*-Butylation Reagents

Other Alkylation Reagents

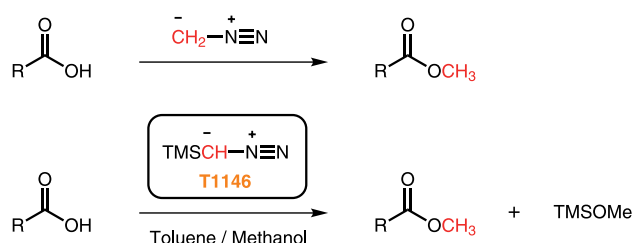
Alkylation Reagents for Ester Synthesis

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.¹⁾ 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.

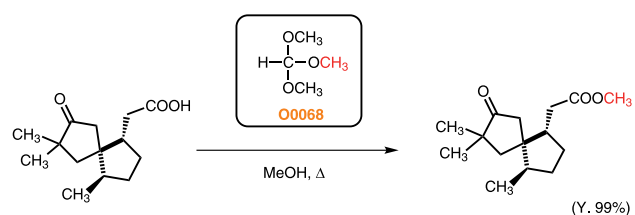


As other traditional synthetic method, the methylation reaction of carboxylic acids is also known using *in situ* generated diazomethane. This reaction proceeds fast under neutral condition. However, since there are several reports on the explosive and cancer-causing property of diazomethane, trimethylsilyldiazomethane – hexane solution (**T1146**), which is less explosive, has been used as an alternative to diazomethane in recent years.²⁾

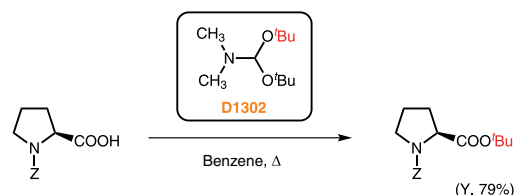


In addition to these reactions above, various kinds of synthetic methods for ester synthesis by alkylating carboxylic acids have been also reported as below.

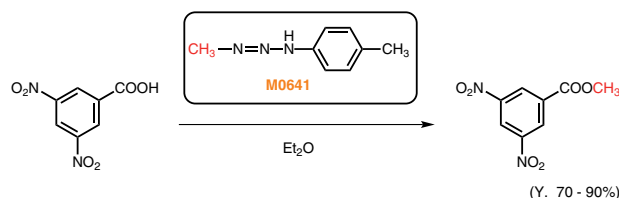
1. Alkylation of Carboxylic Acids using Orthoesters³⁾



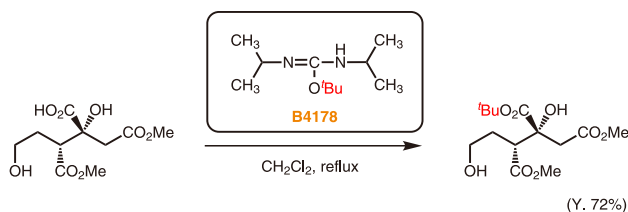
2. Alkylation of Carboxylic Acids using *N,N*-Dimethylformamide Dialkyl Acetals⁴⁾



3. Alkylation of Carboxylic Acids using Triazene Derivatives⁵⁾



4. Alkylation of Carboxylic Acids using *O*-Dialkylisoureas⁶⁾

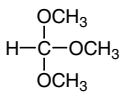
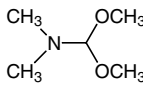
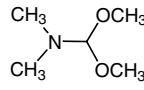
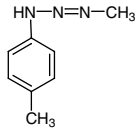
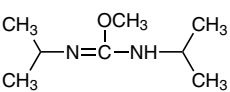
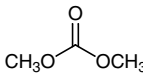
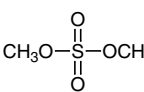
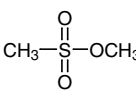
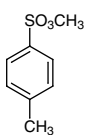
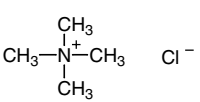
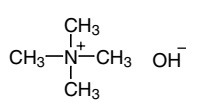
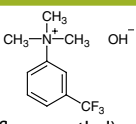
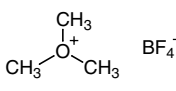
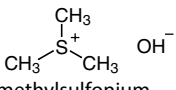
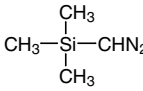
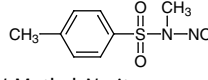
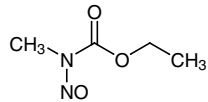
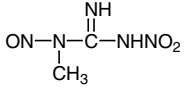
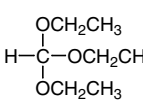
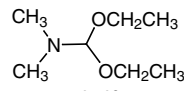
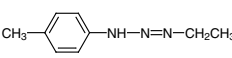


TCI offers a variety of alkylation reagents for ester synthesis other than the reagents above. All the products are listed as below.

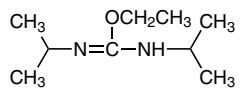
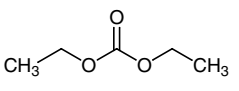
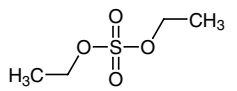
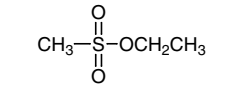
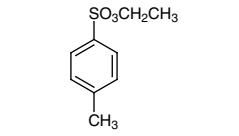
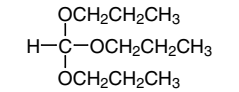
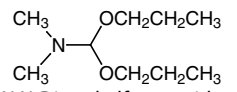
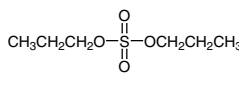
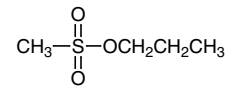
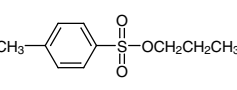
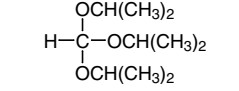
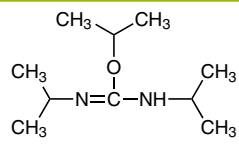
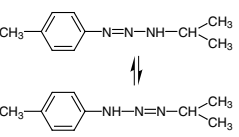
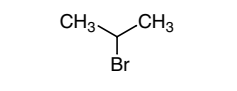
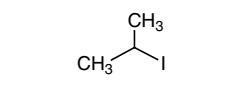
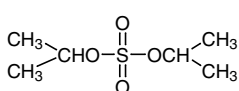
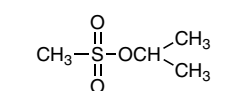
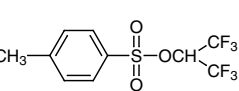
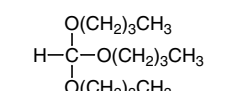
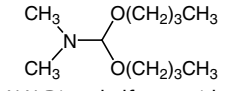
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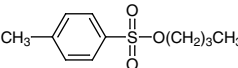
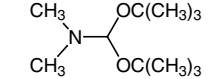
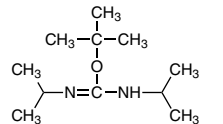
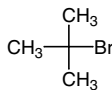
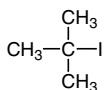
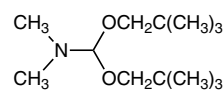
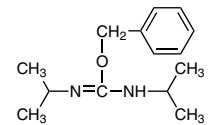
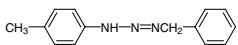
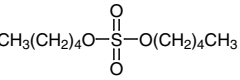
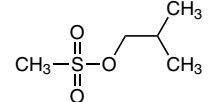
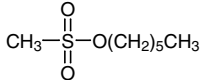
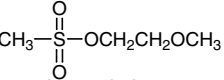
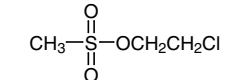
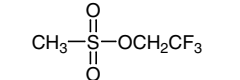
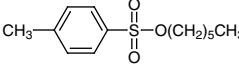
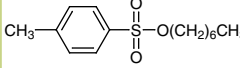
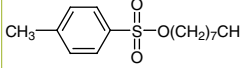
- 1) E. Fischer, A. Speier, *Ber.* **1895**, 28, 3252.
- 2) T. Aoyama, T. Shioiri, *Tetrahedron Lett.* **1980**, 21, 46.
- 3) M. T. Crimmins, J. A. DeLoach, *J. Am. Chem. Soc.* **1986**, 108, 800.
- 4) U. Widmer, *Synthesis* **1983**, 135.
- 5) E. H. White, A. A. Baum, D. E. Eitel, *Org. Synth. Coll.* **1973**, 5, 797.
- 6) F. Calo, J. Richardson, A. G. M. Barrett, *J. Org. Chem.* **2008**, 73, 9692.

Methylation Reagents

<p>X0041 25mL 100mL 500mL</p> <p>Hydrogen Chloride - Methanol Reagent (5-10%) CAS RN: 7647-01-0</p>	<p>X0038 1set</p> <p>Hydrogen Chloride - Methanol Reagent (5-10%) (1mLx10) CAS RN: 7647-01-0</p>	<p>X0033 1set</p> <p>Boron Trichloride - Methanol Reagent (5-10%) CAS RN: 36254-91-8</p>					
<p>X0036 1set</p> <p>Boron Trifluoride - Methanol Reagent (10-20%) CAS RN: 373-57-9</p>	<p>O0068 25mL 500mL</p>  <p>Trimethyl Orthoformate CAS RN: 149-73-5</p>	<p>D2071 25mL</p>  <p><i>N,N</i>-Dimethylformamide Dimethyl Acetal CAS RN: 4637-24-5</p>	<p>D1332 1set</p>  <p><i>N,N</i>-Dimethylformamide Dimethyl Acetal (0.5mLx10) CAS RN: 4637-24-5</p>	<p>M0641 1g 25g</p>  <p>1-Methyl-3-<i>p</i>-tolyltriazene CAS RN: 21124-13-0]</p>			
<p>D4587 5mL</p>  <p><i>N,N'</i>-Diisopropyl-<i>O</i>-methylisourea CAS RN: 54648-79-2</p>	<p>I0060 10mL 100mL 300mL</p> <p>CH₃I</p> <p>Iodomethane (stabilized with Copper chip) CAS RN: 74-88-4</p>	<p>C0053 25mL 100mL 500mL</p>  <p>Dimethyl Carbonate CAS RN: 616-38-6</p>	<p>D0797 25g 500g</p>  <p>Dimethyl Sulfate CAS RN: 77-78-1</p>	<p>M0369 25g 100g</p>  <p>Methyl Methanesulfonate CAS RN: 66-27-3</p>			
<p>T0269 25g 500g</p>  <p>Methyl <i>p</i>-Toluenesulfonate CAS RN: 80-48-8</p>	<p>T0136 25g 500g</p>  <p>Tetramethylammonium Chloride CAS RN: 75-57-0</p>	<p>T0676 25mL 100mL 500mL</p>  <p>Tetramethylammonium Hydroxide (10% in Methanol) CAS RN: 75-59-2</p>	<p>T0961 25mL</p>  <p>3-(Trifluoromethyl)-phenyltrimethylammonium Hydroxide (5% in Methanol) CAS RN: 68254-41-1</p>	<p>T1507 5g 25g</p>  <p>Trimethyloxonium Tetrafluoroborate CAS RN: 420-37-1</p>			
<p>T1576 5mL 25mL</p>  <p>Trimethylsulfonium Hydroxide (0.2mol/L in Methanol) CAS RN: 17287-03-5</p>							
<p>Methylation Reagents (Diazomethane Precursors & Equivalents)</p>					<p>T1146 10mL 25mL 100mL</p>  <p>Trimethylsilyldiazomethane (ca. 10% in Hexane, ca. 0.6mol/L) CAS RN: 18107-18-1</p>	<p>T0323 25g 500g</p>  <p><i>N</i>-Methyl-<i>N</i>-nitroso-<i>p</i>-toluenesulfonamide CAS RN: 80-11-5</p>	<p>N0265 5g 25g</p>  <p><i>N</i>-Methyl-<i>N</i>-nitrosourethane CAS RN: 615-53-2</p>
<p>M0527 5g 25g</p>  <p>1-Methyl-3-nitro-1-nitrosoguanidine (wetted with ca. 50% Water, containing 5g on a dry weight basis) CAS RN: 70-25-7</p>							
<p>Ethylation Reagents</p>					<p>O0066 25mL 500mL</p>  <p>Triethyl Orthoformate CAS RN: 122-51-0</p>	<p>D1294 5mL 25mL</p>  <p><i>N,N</i>-Dimethylformamide Diethyl Acetal CAS RN: 1188-33-6</p>	<p>E0292 1g</p>  <p>1-Ethyl-3-<i>p</i>-tolyltriazene CAS RN: 50707-40-9</p>

Alkylation Reagents for Ester Synthesis

E1058 5mL 25mL  O-Ethyl-N,N'-diisopropylisourea CAS RN: 60683-30-9	B0588 25g 500g $\text{CH}_3\text{CH}_2\text{Br}$ Bromoethane CAS RN: 74-96-4	I0058 25g 100g 500g $\text{CH}_3\text{CH}_2\text{I}$ Iodoethane (stabilized with Copper chip) CAS RN: 75-03-6	C0041 25g 500g  Diethyl Carbonate CAS RN: 105-58-8	D0525 25mL 500mL  Diethyl Sulfate CAS RN: 64-67-5	
M0607 25g 100g  Ethyl Methanesulfonate CAS RN: 62-50-0	T0268 25g 500g  Ethyl <i>p</i> -Toluenesulfonate CAS RN: 80-40-0	<div style="background-color: #4CAF50; color: white; padding: 10px; text-align: center;"> <h3>Propylation & Isopropylation Reagents</h3> </div>			
X0037 1set Boron Trifluoride - Propanol Reagent (10-20%) (1mLx10) CAS RN: 762-48-1	O0259 25mL 500mL  Tripropyl Orthoformate CAS RN: 621-76-1				D1301 5mL 25mL  N,N-Dimethylformamide Dipropyl Acetal CAS RN: 6006-65-1]
B0638 25g 500g $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$ Propyl Bromide CAS RN: 106-94-5	I0068 25g 100g 500g $\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$ Propyl Iodide CAS RN: 107-08-4	D1638 25g 500g  Dipropyl Sulfate CAS RN: 598-05-0	P1844 5g 25g  Propyl Methanesulfonate CAS RN: 1912-31-8	T0726 25mL 500mL  Propyl <i>p</i> -Toluenesulfonate CAS RN: 599-91-7	
X0035 1set Boron Trifluoride - Isopropyl Alcohol Reagent (10-20%) (1mLx10) CAS RN: 676-65-3	O0215 25mL  Triisopropoxymethane CAS RN: 4447-60-3	T3123 5mL 25mL  O,N,N'-Triisopropylisourea CAS RN: 63460-32-2	I0280 1g  1-Isopropyl-3- <i>p</i> -tolyltriazene CAS RN: 50707-41-0	B0639 25g 500g  Isopropyl Bromide CAS RN: 75-26-3	
I0069 25g 100g 500g  Isopropyl Iodide CAS RN: 75-30-9	D2954 5g 25g  Diisopropyl Sulfate CAS RN: 2973-10-6	I0914 1g 5g  Isopropyl Methanesulfonate CAS RN: 926-06-7	H1281 5g 25g  1,1,1,3,3,3-Hexafluoroisopropyl <i>p</i> -Toluenesulfonate CAS RN: 67674-48-0		
<div style="background-color: #4CAF50; color: white; padding: 10px; text-align: center;"> <h3>Butylation & tert-Butylation Reagents</h3> </div>			X0039 1set Hydrogen Chloride - Butanol Reagent (5-10%) (1mLx10) CAS RN: 647-01-0	X0034 1set Boron Trifluoride - Butanol Reagent (10-20%) (1mLx10) CAS RN: 692-39-7	O0269 25mL  Tributyl Orthoformate CAS RN: 588-43-2
			D1302 5mL 25mL  N,N-Dimethylformamide Dibutyl Acetal CAS RN: 18503-90-7	B0560 25g 500g $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$ Butyl Bromide CAS RN: 109-65-9	I0055 25g 500g $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ Butyl Iodide CAS RN: 542-69-8

T0727 25mL 500mL  Butyl <i>p</i> -Toluenesulfonate CAS RN: 778-28-9	D1303 5mL 25mL  <i>N,N</i> -Dimethylformamide Di- <i>tert</i> -butyl Acetal CAS RN: 36805-97-7	B4178 1g 5g  <i>O-tert</i> -Butyl- <i>N,N'</i> -diisopropylisourea CAS RN: 71432-55-8	B0617 25g 100g 500g  <i>tert</i> -Butyl Bromide CAS RN: 507-19-7	B1072 25g  <i>tert</i> -Butyl Iodide CAS RN: 558-17-8
Other Alkylation Reagents		X0032 1set Boron Trichloride - 2-Chloroethanol Reagent (5-10%) (1mLx10) CAS RN: 75507-65-2	D1595 5mL 25mL  <i>N,N</i> -Dimethylformamide Dineopentyl Acetal CAS RN: 4909-78-8	B4480 1mL 5mL  <i>O</i> -Benzyl- <i>N,N'</i> -diisopropylisourea CAS RN: 2978-10-1
B0949 1g 25g  1-Benzyl-3- <i>p</i> -tolyltriazeno CAS RN: 17683-09-9	D2955 5g  Diamyl Sulfate CAS RN: 5867-98-1	I1062 1g 5g  Isobutyl Methanesulfonate CAS RN: 16156-53-9	H1282 5g 25g  Hexyl Methanesulfonate CAS RN: 16156-50-6	M1446 5g 25g  2-Methoxyethyl Methanesulfonate CAS RN: 16427-44-4
C2231 5g  2-Chloroethyl Methanesulfonate CAS RN: 3570-58-9	M1193 5g 25g  2,2,2-Trifluoroethyl Methanesulfonate CAS RN: 25236-64-0	T0883 25g 500g  Hexyl <i>p</i> -Toluenesulfonate CAS RN: 3839-35-8	T0884 25g 500g  Heptyl <i>p</i> -Toluenesulfonate CAS RN: 24767-82-6	T0885 25g 500g  <i>n</i> -Octyl <i>p</i> -Toluenesulfonate CAS RN: 3386-35-4

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