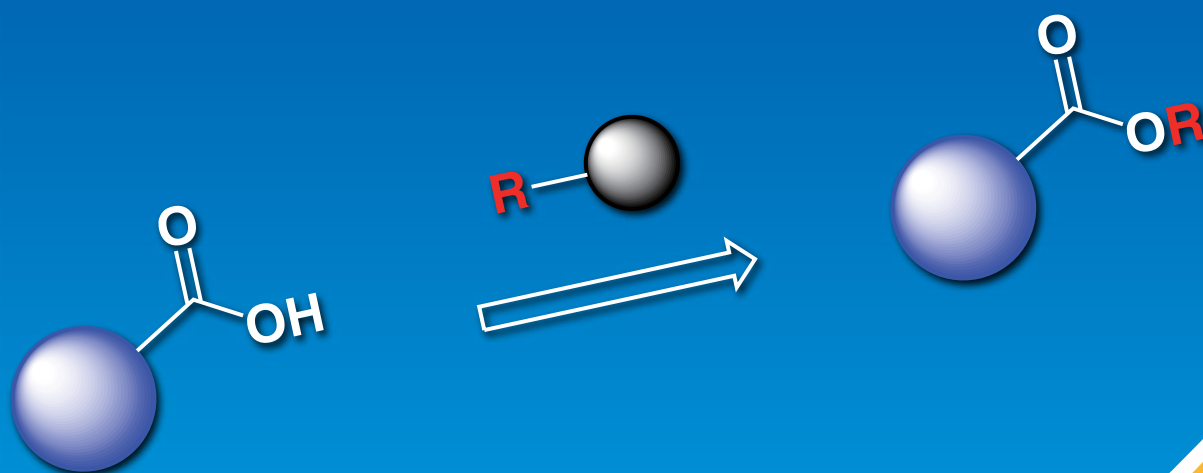


Alkylation Reagents for Ester Synthesis



Methylation Reagents

Methylation Reagents (Diazomethane Precursors/Equivalents)

Ethylation Reagents

Propylation & Isopropylation Reagents

Butylation & *tert*-Butylation Reagents

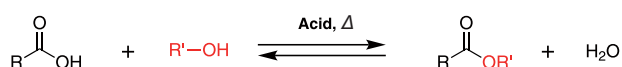
Benzylation Reagents

Other Alkylation Reagents

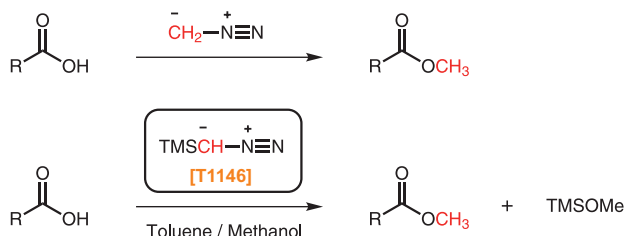
Alkylation Reagents for Ester Synthesis

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.

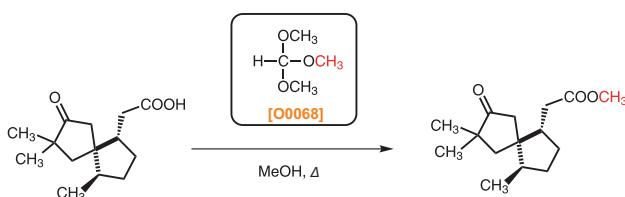


As other traditional synthetic method, the methylation reaction of carboxylic acids is also known using *in situ* generated diazomethane. This reaction proceeds fast under neutral condition. However, since there are several reports on the explosive and cancer-causing property of diazomethane, trimethylsilyldiazomethane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

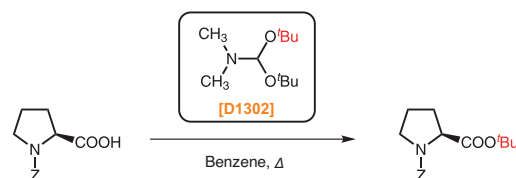


In addition to these reactions above, various kinds of synthetic methods for ester synthesis by alkylating carboxylic acids have been also reported as below.

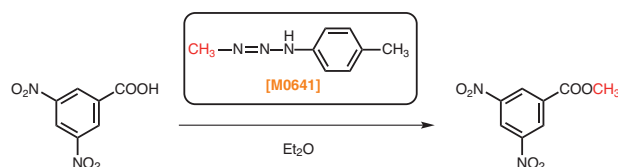
1. Alkylation of Carboxylic Acids using Orthoesters³⁾



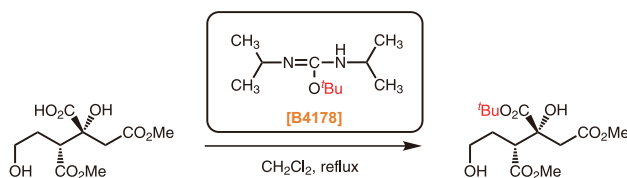
2. Alkylation of Carboxylic Acids using *N,N*-Dimethylformamide Dialkyl Acetals⁴⁾



3. Alkylation of Carboxylic Acids using Triazene Derivatives⁵⁾



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

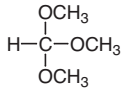
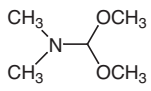
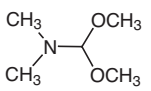
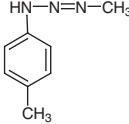
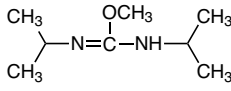
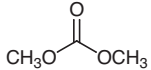
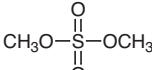
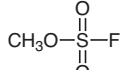
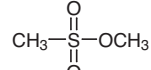
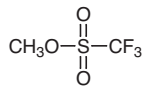
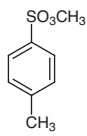
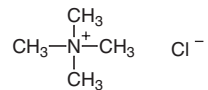
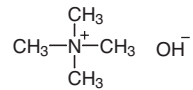
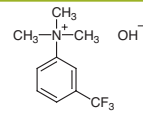
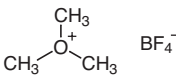
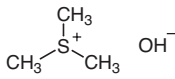


TCI offers a variety of alkylation reagents for ester synthesis other than the reagents above. All the products are listed as below.

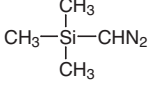
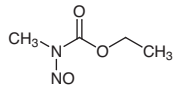
References

- 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.

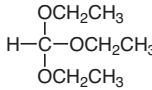
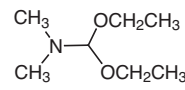
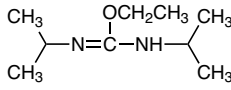
Methylation Reagents

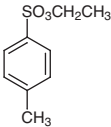
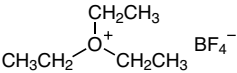
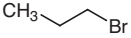
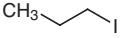
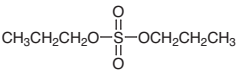
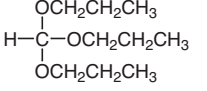
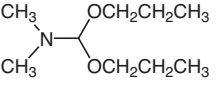
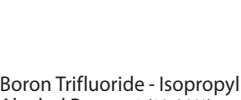
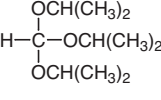
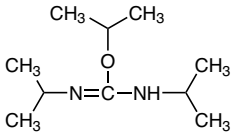
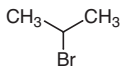
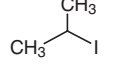
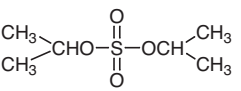
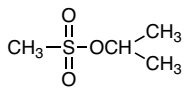
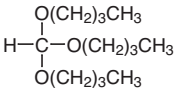
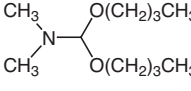
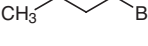
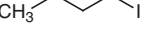
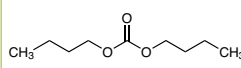
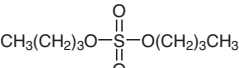
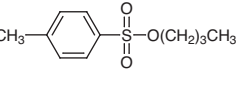
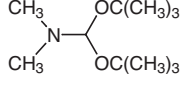
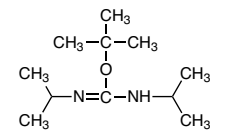
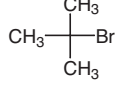
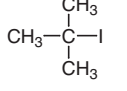
Methylation Reagents		X0041	25mL 100mL 500mL	X0033	1set	X0036	1set
		Hydrogen Chloride - Methanol Reagent (5-10%) CAS RN: 7647-01-0		Boron Trichloride - Methanol Reagent (5-10%) CAS RN: 36254-91-8		Boron Trifluoride - Methanol Reagent (10-20%) CAS RN: 373-57-9	
O0068	25mL 500mL	D2071	25mL	D1332	1set	M0641	1g 25g
	Trimethyl Orthoformate CAS RN: 149-73-5		<i>N,N</i> -Dimethylformamide Dimethyl Acetal CAS RN: 4637-24-5		<i>N,N</i> -Dimethylformamide Dimethyl Acetal (0.5mLx10) CAS RN: 4637-24-5		1-Methyl-3- <i>p</i> -tolyltriazene CAS RN: 21124-13-0
	<i>N,N'</i> -Diisopropyl- <i>O</i> -methylisourea CAS RN: 54648-79-2						
I0060	10mL 100mL 300mL	C0053	25mL 100mL 500mL	D0797	25g 500g	F0238	5g 25g
	Iodomethane CAS RN: 74-88-4		Dimethyl Carbonate CAS RN: 616-38-6		Dimethyl Sulfate CAS RN: 77-78-1		Methyl Fluorosulfonate CAS RN: 421-20-5
	Methyl Methanesulfonate CAS RN: 66-27-3						
T2029	5g 25g	T0269	25g 500g	T0136	25g 500g	T0676	25mL 100mL 500mL
	Methyl Triflate CAS RN: 333-27-7		Methyl <i>p</i> -Toluenesulfonate CAS RN: 80-48-8		Tetramethylammonium Chloride CAS RN: 75-57-0		Tetramethylammonium Hydroxide (10% in Methanol) CAS RN: 75-59-2
	3-(Trifluoromethyl)- phenyltrimethylammonium Hydroxide (5% in Methanol) CAS RN: 68254-41-1						
T1507	5g 25g	T1576	5mL 25mL				
	Trimethyloxonium Tetrafluoroborate CAS RN: 420-37-1		Trimethylsulfonium Hydroxide (0.2mol/L in Methanol) CAS RN: 17287-03-5				

Methylation Reagents (Diazomethane Precursors & Equivalents)

T1146 10mL 25mL 100mL  Trimethylsilyldiazomethane (ca. 10% in Hexane, ca. 0.6mol/L) CAS RN: 18107-18-1	N0265 5g 25g  <i>N</i> -Methyl- <i>N</i> -nitrosourea CAS RN: 615-53-2
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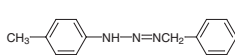
Ethylation Reagents

Ethylation Reagents			O0066 25mL 500mL  Triethyl Orthoformate CAS RN: 122-51-0	D1294 5mL 25mL  <i>N,N</i> -Dimethylformamide Diethyl Acetal CAS RN: 1188-33-6	E1058 5mL 25mL  <i>O</i> -Ethyl- <i>N,N'</i> -diisopropylisourea CAS RN: 60683-30-9
B0588 25g 500g 					

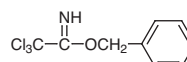
T026825g 500g  Ethyl <i>p</i>-Toluenesulfonate CAS RN: 80-40-0	T1606100mL  Triethyloxonium Tetrafluoroborate (15% in Dichloromethane, ca. 1mol/L) CAS RN: 368-39-8			
Propylation & Isopropylation Reagents				
B063825g 500g  Propyl Bromide CAS RN: 106-94-5	I006825g 100g 500g  Propyl Iodide CAS RN: 107-08-4	D163825g 500g  Dipropyl Sulfate CAS RN: 598-05-0	O025925mL  Tripropyl Orthoformate CAS RN: 621-76-1	D13015mL 25mL  <i>N,N</i>-Dimethylformamide Dipropyl Acetal CAS RN: 6006-65-1
X00351set  Boron Trifluoride - Isopropyl Alcohol Reagent (10-20%) (1mLx10) CAS RN: 676-65-3	O021525mL  Triisopropoxymethane CAS RN: 4447-60-3	T31235mL 25mL  <i>O,N'</i>-Triisopropylisourea CAS RN: 63460-32-2	B063925g 500g  Isopropyl Bromide CAS RN: 75-26-3	I006925g 100g 500g  Isopropyl Iodide CAS RN: 75-30-9
D29545g 25g  Diisopropyl Sulfate CAS RN: 2973-10-6	I09141g 5g  Isopropyl Methanesulfonate CAS RN: 926-06-7	X00391set  Hydrogen Chloride - Butanol Reagent (5-10%) (1mLx10) CAS RN: 7647-01-0	X00341set  Boron Trifluoride - Butanol Reagent (10-20%) (1mLx10) CAS RN: 692-39-7	O026925mL  Tributyl Orthoformate CAS RN: 588-43-2
Butylation & <i>tert</i>-Butylation Reagents				
D13025mL 25mL  <i>N,N</i>-Dimethylformamide Dibutyl Acetal CAS RN: 18503-90-7	B056025g 500g  Butyl Bromide CAS RN: 109-65-9	I005525g 500g  Butyl Iodide CAS RN: 542-69-8	C00405g 25g  Dibutyl Carbonate CAS RN: 542-52-9	D163325g 500g  Dibutyl Sulfate CAS RN: 625-22-9
T072725mL 500mL  Butyl <i>p</i>-Toluenesulfonate CAS RN: 778-28-9	D13035mL 25mL  <i>N,N</i>-Dimethylformamide Di-<i>tert</i>-butyl Acetal CAS RN: 36805-97-7	B41781g 5g  <i>O-tert</i>-Butyl-<i>N,N'</i>-diisopropylisourea CAS RN: 71432-55-8	B061725g 100g 500g  <i>tert</i>-Butyl Bromide CAS RN: 507-19-7	B107225g  <i>tert</i>-Butyl Iodide CAS RN: 558-17-8

Benzylation Reagents

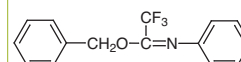
B0949 1g 25g

1-Benzyl-3-*p*-tolyltriazene
CAS RN: 17683-09-9

B1483 25g

Benzyl
2,2,2-Trichloroacetimidate
CAS RN: 81927-55-1

B3234 1g 5g

Benzyl 2,2,2-Trifluoro-*N*-phenylacetimidate
CAS RN: 952057-61-3

B0412 25g 500g

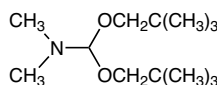
Benzyl Chloride
CAS RN: 100-44-7

B0411 25g 100g 500g

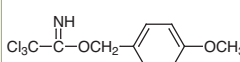
Benzyl Bromide
CAS RN: 100-39-0

Other Alkylation Reagents

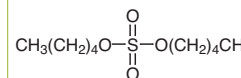
D1595 5mL 25mL

*N,N*-Dimethylformamide
Dineopentyl Acetal
CAS RN: 4909-78-8

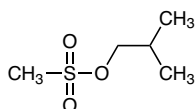
M2016 5g 25g

4-Methoxybenzyl
2,2,2-Trichloroacetimidate
CAS RN: 89238-99-3

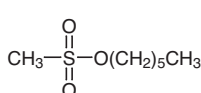
D2955 5g

Diamyl Sulfate
CAS RN: 5867-98-1

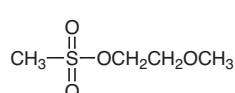
I1062 1g 5g

Isobutyl Methanesulfonate
CAS RN: 16156-53-9

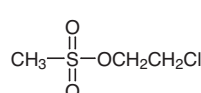
H1282 5g 25g

Hexyl Methanesulfonate
CAS RN: 16156-50-6

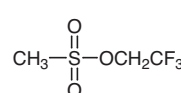
M1446 5g 25g

2-Methoxyethyl
Methanesulfonate
CAS RN: 16427-44-4

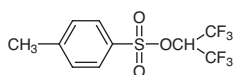
C2231 5g

2-Chloroethyl
Methanesulfonate
CAS RN: 3570-58-9

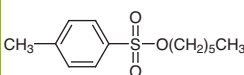
M1193 5g 25g

2,2,2-Trifluoroethyl
Methanesulfonate
CAS RN: 25236-64-0

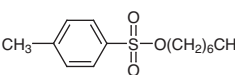
H1281 5g 25g

1,1,1,3,3,3-Hexafluoroisopropyl
p-Toluenesulfonate
CAS RN: 67674-48-0

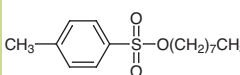
T0883 25g 500g

Hexyl *p*-Toluenesulfonate
CAS RN: 3839-35-8

T0884 25g 500g

Heptyl *p*-Toluenesulfonate
CAS RN: 24767-82-6

T0885 25g 500g

*n*-Octyl *p*-Toluenesulfonate
CAS RN: 3386-35-4

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E-mail : Sales-UK@TCIchemicals.com

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E-mail : globalbusiness@TCIchemicals.com

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