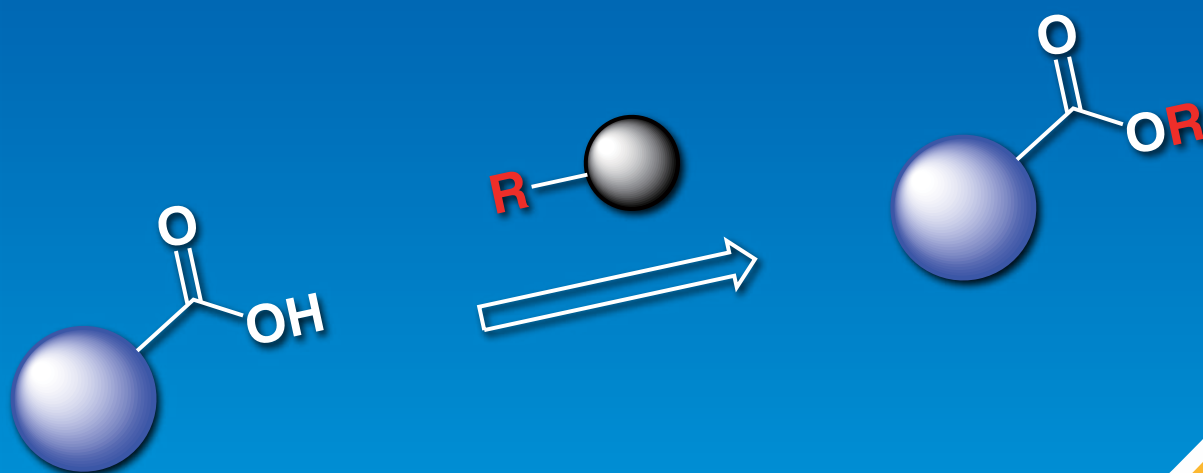


Alkylation Reagents for Ester Synthesis



Methylation Reagents

Methylation Reagents (Diazomethane Precursors/Equivalents)

Ethylation Reagents

Propylation & Isopropylation Reagents

Butylation & *tert*-Butylation Reagents

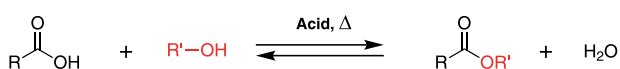
Benzylation Reagents

Other Alkylation Reagents

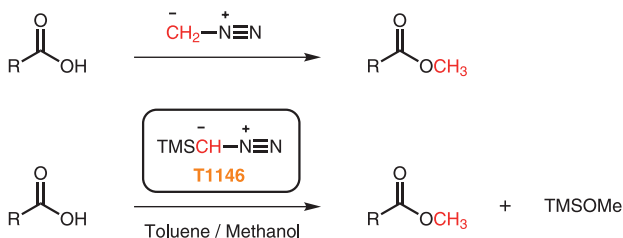
Alkylation Reagents for Ester Synthesis

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.

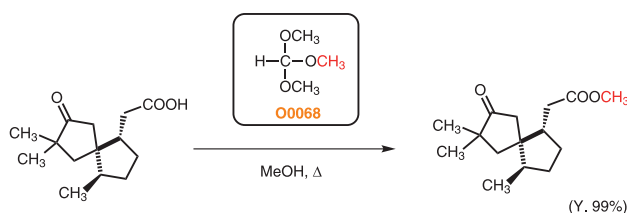


As other traditional synthetic method, the methylation reaction of carboxylic acids is also known using *in situ* generated diazomethane. This reaction proceeds fast under neutral condition. However, since there are several reports on the explosive and cancer-causing property of diazomethane, trimethylsilyldiazomethane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

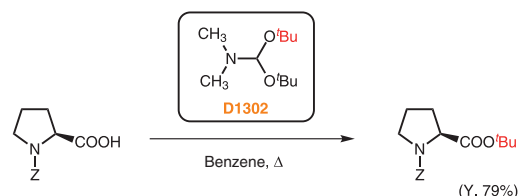


In addition to these reactions above, various kinds of synthetic methods for ester synthesis by alkylating carboxylic acids have been also reported as below.

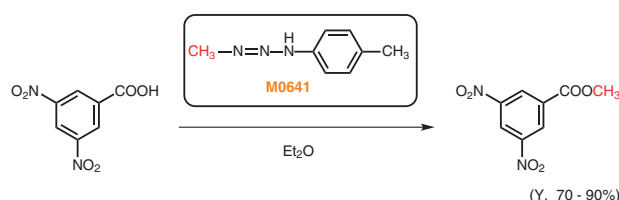
1. Alkylation of Carboxylic Acids using Orthoesters³⁾



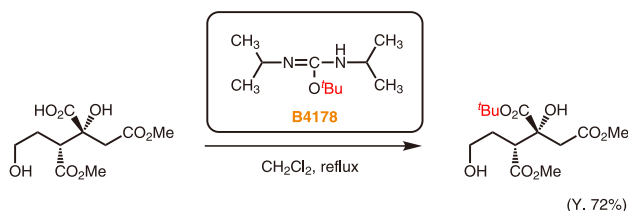
2. Alkylation of Carboxylic Acids using *N,N*-Dimethylformamide Dialkyl Acetals⁴⁾



3. Alkylation of Carboxylic Acids using Triazene Derivatives⁵⁾



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

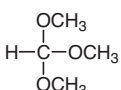
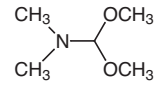
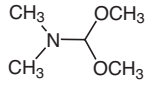
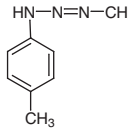
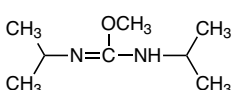
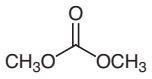
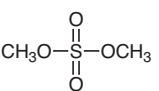
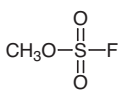
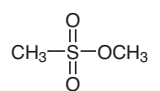
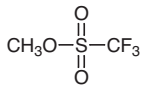
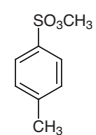
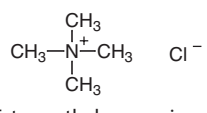
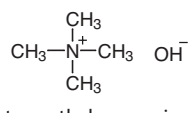
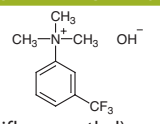
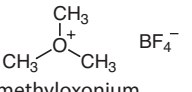
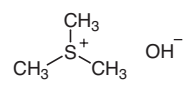


TCI offers a variety of alkylation reagents for ester synthesis other than the reagents above. All the products are listed as below.

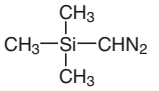
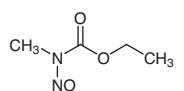
References

- 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.

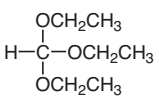
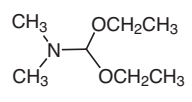
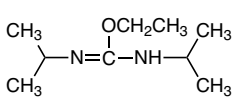
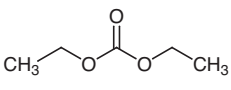
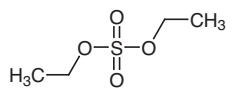
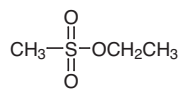
Methylation Reagents

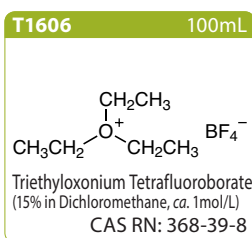
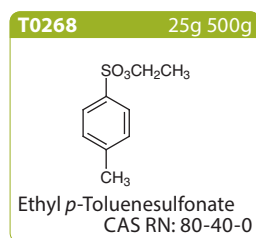
Methylation Reagents		X0041 25mL 100mL 500mL Hydrogen Chloride - Methanol Reagent (5-10%) CAS RN: 7647-01-0	X0033 1set Boron Trichloride - Methanol Reagent (5-10%) CAS RN: 36254-91-8	X0036 1set Boron Trifluoride - Methanol Reagent (10-20%) CAS RN: 373-57-9		
		O0068 25mL 500mL  Trimethyl Orthoformate CAS RN: 149-73-5	D2071 25mL  <i>N,N</i> -Dimethylformamide Dimethyl Acetal CAS RN: 4637-24-5	D1332 1set  <i>N,N</i> -Dimethylformamide Dimethyl Acetal (0.5mLx10) CAS RN: 4637-24-5	M0641 1g 25g  1-Methyl-3- <i>p</i> -tolyltriazene CAS RN: 21124-13-0	D4587 5mL  <i>N,N'</i> -Diisopropyl- <i>O</i> -methylisourea CAS RN: 54648-79-2
		I0060 10mL 100mL 300mL CH ₃ I Iodomethane CAS RN: 74-88-4	C0053 25mL 100mL 500mL  Dimethyl Carbonate CAS RN: 616-38-6	D0797 25g 500g  Dimethyl Sulfate CAS RN: 77-78-1	F0238 5g 25g  Methyl Fluorosulfonate CAS RN: 421-20-5	M0369 25g 100g  Methyl Methanesulfonate CAS RN: 66-27-3
		T2029 5g 25g  Methyl Triflate CAS RN: 333-27-7	T0269 25g 500g  Methyl <i>p</i> -Toluenesulfonate CAS RN: 80-48-8	T0136 25g 500g  Tetramethylammonium Chloride CAS RN: 75-57-0	T0676 25mL 100mL 500mL  Tetramethylammonium Hydroxide (10% in Methanol) CAS RN: 75-59-2	T0961 25mL 100mL  3-(Trifluoromethyl)-phenyltrimethylammonium Hydroxide (5% in Methanol) CAS RN: 68254-41-1
		T1507 5g 25g  Trimethyloxonium Tetrafluoroborate CAS RN: 420-37-1	T1576 5mL 25mL  Trimethylsulfonium Hydroxide (0.2mol/L in Methanol) CAS RN: 17287-03-5			

Methylation Reagents (Diazomethane Precursors & Equivalents)

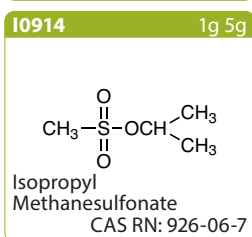
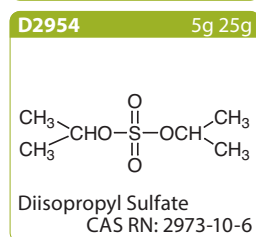
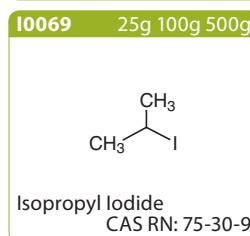
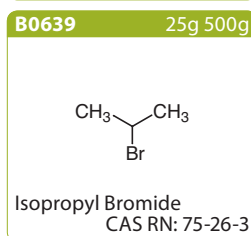
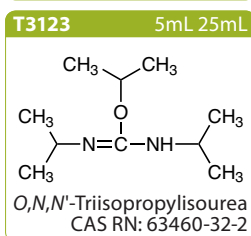
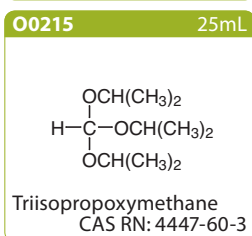
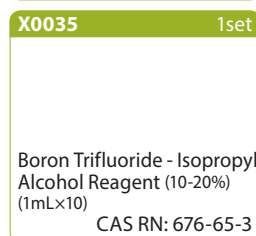
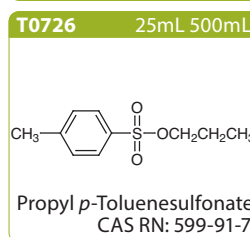
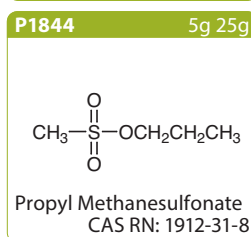
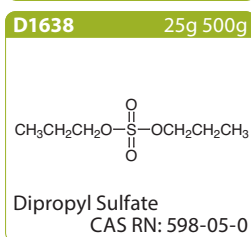
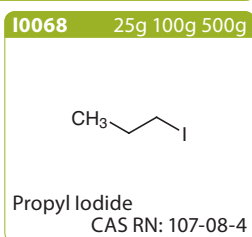
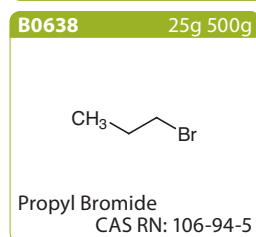
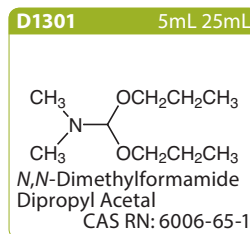
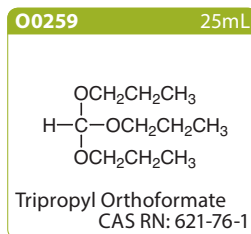
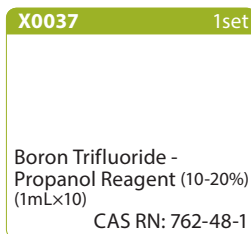
T1146 10mL 25mL 100mL  Trimethylsilyldiazomethane (ca. 10% in Hexane, ca. 0.6mol/L) CAS RN: 18107-18-1	N0265 5g 25g  <i>N</i> -Methyl- <i>N</i> -nitrosourea CAS RN: 615-53-2
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Ethylation Reagents

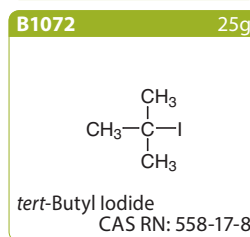
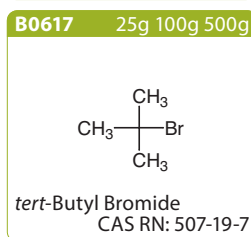
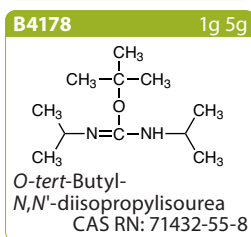
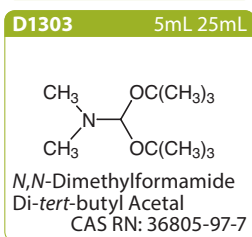
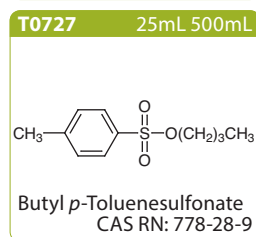
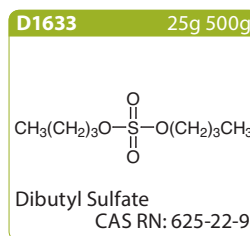
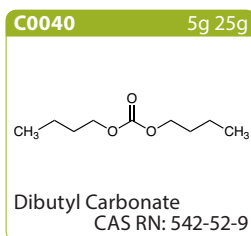
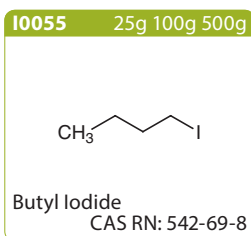
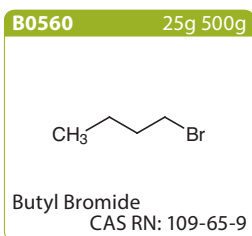
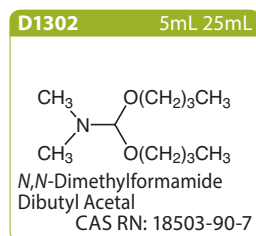
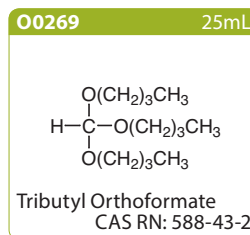
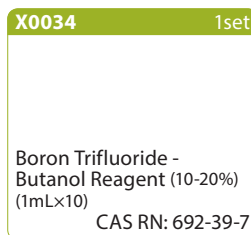
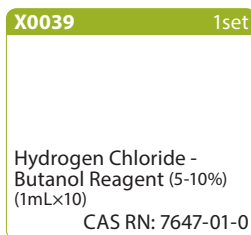
Ethylation Reagents		O0066 25mL 500mL  Triethyl Orthoformate CAS RN: 122-51-0	D1294 5mL 25mL  <i>N,N</i> -Dimethylformamide Diethyl Acetal CAS RN: 1188-33-6	E1058 5mL 25mL  <i>O</i> -Ethyl- <i>N,N'</i> -diisopropylisourea CAS RN: 60683-30-9		
		B0588 25g 500g CH ₃ CH ₂ Br Bromoethane CAS RN: 74-96-4	I0058 25g 100g 500g CH ₃ CH ₂ 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



Propylation & Isopropylation Reagents

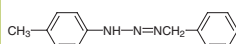


Butylation & tert-Butylation Reagents

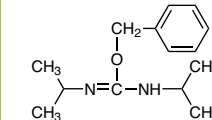


Benzylation Reagents

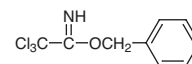
B0949 1g 25g

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

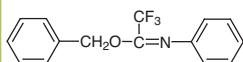
B4480 1mL 5mL

O-Benzyl-*N,N'*-diisopropylisourea
CAS RN: 2978-10-1

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 250g

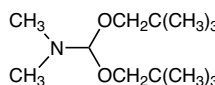
Benzyl Chloride
CAS RN: 100-44-7

B0411 25g 100g 500g

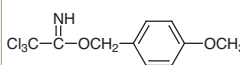
Benzyl Bromide
CAS RN: 100-39-0

Other Alkylation Reagents

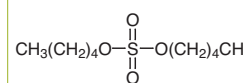
D1595 5mL 25mL

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

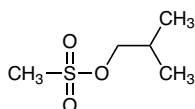
M2016 5g 25g

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

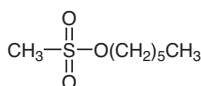
D2955 5g

Diamyl Sulfate
CAS RN: 5867-98-1

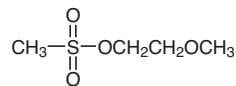
I1062 1g 5g

Isobutyl Methanesulfonate
CAS RN: 16156-53-9

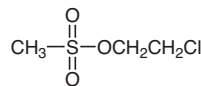
H1282 5g 25g

Hexyl Methanesulfonate
CAS RN: 16156-50-6

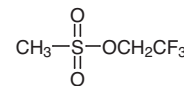
M1446 5g 25g

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

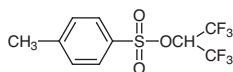
C2231 5g

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

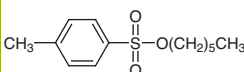
M1193 5g 25g

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

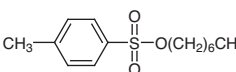
H1281 5g 25g

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

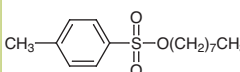
T0883 25g 500g

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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