CAS SciFinder^{n}

Task History

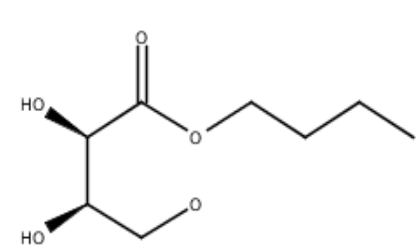
Initiating Search

July 17, 2021, 8:52AM

Substances:

Filtered By:

Structure Match:	**Similarity**
Similarity:	**85-89, 90-94, 95-98, >=99**
Number of Components:	**1**



Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters	**Substances**	View Results

CAS SciFinder^{n}

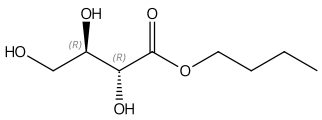
Substances (42)

View in SciFinder^{n}

1

Similarity Score: **100**

898285-31-9



Absolute stereochemistry shown

$C_8H_{16}O_5$

Butyl (2*R*,3*R*)-2,3,4-trihydroxybutanoate

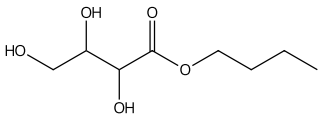
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	192.21	-
Melting Point (Experimental)	62-64 °C	-
Boiling Point (Predicted)	337.7±21.0 °C	Press: 760 Torr
Density (Predicted)	1.221±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.14±0.20	Most Acidic Temp: 25 °C
Experimental Properties		

2

Similarity Score: **100**

887617-89-2



$C_8H_{16}O_5$

Butyl 2,3,4-trihydroxybutanoate

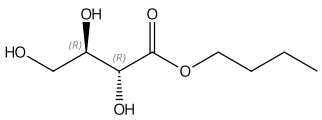
1 Reference | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	192.21	-
Boiling Point (Predicted)	337.7±21.0 °C	Press: 760 Torr
Density (Predicted)	1.221±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.14±0.20	Most Acidic Temp: 25 °C

3

Similarity Score: **100**

74421-62-8



Relative stereochemistry shown

$C_8H_{16}O_5$

rel-Butyl (2*R*,3*R*)-2,3,4-trihydroxybutanoate

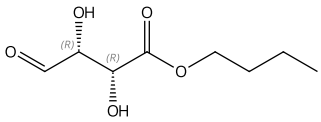
0 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	192.21	-
Boiling Point (Predicted)	337.7±21.0 °C	Press: 760 Torr
Density (Predicted)	1.221±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.14±0.20	Most Acidic Temp: 25 °C

4

Similarity Score: **98**

887618-53-3



Relative stereochemistry shown

$C_8H_{14}O_5$

rel-Butyl (2*R*,3*R*)-2,3-dihydroxy-4-oxobutanoate

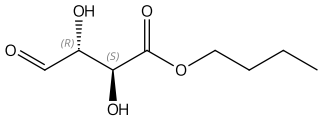
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	190.19	-
Boiling Point (Predicted)	360.8±42.0 °C	Press: 760 Torr
Density (Predicted)	1.210±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.82±0.20	Most Acidic Temp: 25 °C

5

Similarity Score: **98**

887618-42-0



Relative stereochemistry shown

$C_8H_{14}O_5$

rel-Butyl (2*R*,3*S*)-2,3-dihydroxy-4-oxobutanoate

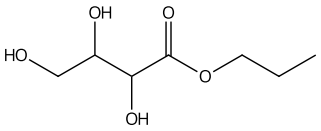
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	190.19	-
Boiling Point (Predicted)	360.8±42.0 °C	Press: 760 Torr
Density (Predicted)	1.210±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.82±0.20	Most Acidic Temp: 25 °C

6

Similarity Score: **94**

887617-87-0



$C_7H_{14}O_5$

Propyl 2,3,4-trihydroxybutanoate

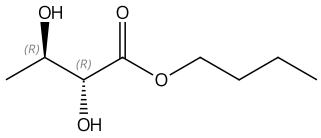
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	178.18	-
Boiling Point (Predicted)	326.0±21.0 °C	Press: 760 Torr
Density (Predicted)	1.265±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.14±0.20	Most Acidic Temp: 25 °C

7

Similarity Score: **93**

2165859-85-6



Absolute stereochemistry shown

$C_8H_{16}O_4$

Butanoic acid, 2,3-dihydroxy-, butyl ester, (2*R*, 3*R*)-

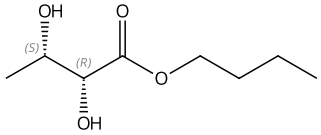
0 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	176.21	-
Boiling Point (Predicted)	283.9±7.0 °C	Press: 760 Torr
Density (Predicted)	1.102±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.72±0.20	Most Acidic Temp: 25 °C

8

Similarity Score: **93**

2165531-03-1



Absolute stereochemistry shown

$C_8H_{16}O_4$

Butanoic acid, 2,3-dihydroxy-, butyl ester, (2*R*, 3*S*)-

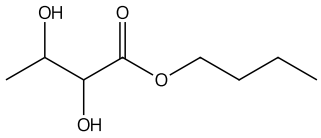
0 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	176.21	-
Boiling Point (Predicted)	283.9±7.0 °C	Press: 760 Torr
Density (Predicted)	1.102±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.72±0.20	Most Acidic Temp: 25 °C

9

Similarity Score: **93**

1823660-59-8



$C_8H_{16}O_4$

Butanoic acid, 2,3-dihydroxy-, butyl ester

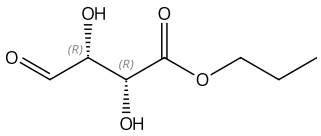
0 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	176.21	-
Boiling Point (Predicted)	283.9±7.0 °C	Press: 760 Torr
Density (Predicted)	1.102±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.72±0.20	Most Acidic Temp: 25 °C

10

Similarity Score: **93**

887618-51-1



Relative stereochemistry shown

$C_7H_{12}O_5$

rel-Propyl (2*R*,3*R*)-2,3-dihydroxy-4-oxobutanoate

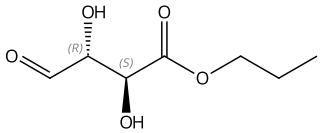
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	176.17	-
Boiling Point (Predicted)	352.0±42.0 °C	Press: 760 Torr
Density (Predicted)	1.252±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.83±0.20	Most Acidic Temp: 25 °C

11

Similarity Score: **93**

887618-40-8



Relative stereochemistry shown

$C_7H_{12}O_5$

rel-Propyl (2*R*,3*S*)-2,3-dihydroxy-4-oxobutanoate

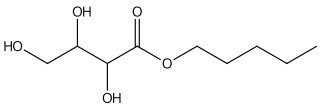
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	176.17	-
Boiling Point (Predicted)	352.0±42.0 °C	Press: 760 Torr
Density (Predicted)	1.252±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.83±0.20	Most Acidic Temp: 25 °C

12

Similarity Score: **89**

887617-90-5



$C_9H_{18}O_5$

Pentyl 2,3,4-trihydroxybutanoate

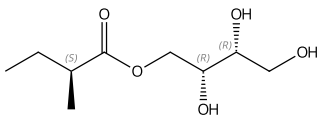
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	206.24	-
Boiling Point (Predicted)	350.1±21.0 °C	Press: 760 Torr
Density (Predicted)	1.186±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.15±0.20	Most Acidic Temp: 25 °C

13

Similarity Score: **88**

910658-45-6



Absolute stereochemistry shown, Rotation (+)

$C_9H_{18}O_5$

(2*R*,3*R*)-2,3,4-Trihydroxybutyl (2*S*)-2-methylbutanoate

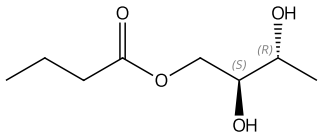
2 References | 1 Reaction | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	206.24	-
Boiling Point (Predicted)	373.5±42.0 °C	Press: 760 Torr
Density (Predicted)	1.183±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.04±0.20	Most Acidic Temp: 25 °C

14

Similarity Score: **88**

2305574-39-2



Absolute stereochemistry shown, Rotation (+)

$C_8H_{16}O_4$

Butanoic acid, (2*S*,3*R*)-2,3-dihydroxybutyl ester

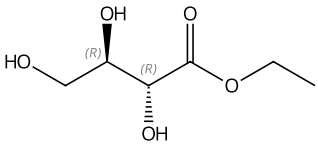
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	176.21	-
Boiling Point (Predicted)	287.9±20.0 °C	Press: 760 Torr
Density (Predicted)	1.102±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.63±0.20	Most Acidic Temp: 25 °C

15

Similarity Score: **88**

910658-47-8



Absolute stereochemistry shown, Rotation (+)

$C_6H_{12}O_5$

Ethyl (2*R*,3*R*)-2,3,4-trihydroxybutanoate

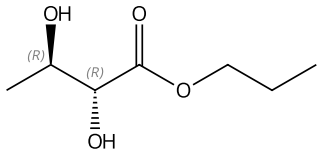
2 References | 1 Reaction | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	164.16	-
Boiling Point (Predicted)	315.4±21.0 °C	Press: 760 Torr
Density (Predicted)	1.320±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.29±0.20	Most Acidic Temp: 25 °C

16

Similarity Score: **88**

1071575-19-3



Absolute stereochemistry shown

$C_7H_{14}O_4$

Propyl (2*R*,3*R*)-2,3-dihydroxybutanoate

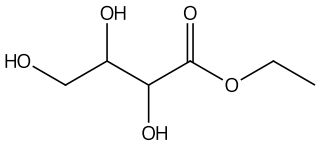
1 Reference | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	162.18	-
Boiling Point (Experimental)	117 °C	Press: 10 Torr
Density (Predicted)	1.131±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.72±0.20	Most Acidic Temp: 25 °C
Experimental Properties		

17

Similarity Score: **88**

887617-86-9



$C_6H_{12}O_5$

Ethyl 2,3,4-trihydroxybutanoate

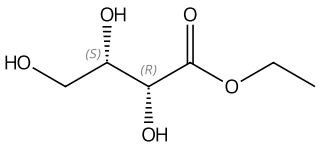
1 Reference | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	164.16	-
Boiling Point (Predicted)	315.4±21.0 °C	Press: 760 Torr
Density (Predicted)	1.320±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.29±0.20	Most Acidic Temp: 25 °C

18

Similarity Score: **88**

115994-88-2



Relative stereochemistry shown

$C_6H_{12}O_5$

Butanoic acid, 2,3,4-trihydroxy-, ethyl ester, (*R**,*S**)-

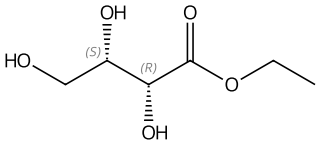
1 Reference | 0 Reactions | 3 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	164.16	-
Boiling Point (Predicted)	315.4±21.0 °C	Press: 760 Torr
Density (Predicted)	1.320±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.29±0.20	Most Acidic Temp: 25 °C

19

Similarity Score: **88**

2165660-15-9



Absolute stereochemistry shown

$C_6H_{12}O_5$

Ethyl (2*R*,3*S*)-2,3,4-trihydroxybutanoate

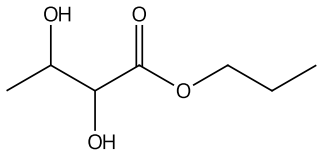
0 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	164.16	-
Boiling Point (Predicted)	315.4±21.0 °C	Press: 760 Torr
Density (Predicted)	1.320±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.29±0.20	Most Acidic Temp: 25 °C

20

Similarity Score: **88**

1823530-30-8



$C_7H_{14}O_4$

Butanoic acid, 2,3-dihydroxy-, propyl ester

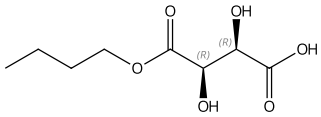
0 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	162.18	-
Boiling Point (Predicted)	268.2±7.0 °C	Press: 760 Torr
Density (Predicted)	1.131±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.72±0.20	Most Acidic Temp: 25 °C

21

Similarity Score: **88**

121536-75-2



Absolute stereochemistry shown

$C_8H_{14}O_6$

Butanedioic acid, 2,3-dihydroxy- (2*R*,3*R*)-, monobutyl ester

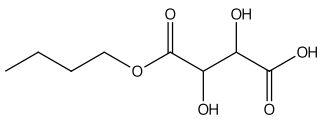
5 References | 1 Reaction | 2 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	206.19	-
Boiling Point (Predicted)	435.7±45.0 °C	Press: 760 Torr
Density (Predicted)	1.334±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.27±0.34	Most Acidic Temp: 25 °C

22

Similarity Score: **88**

856055-26-0



$C_8H_{14}O_6$

4-Butyl 2,3-dihydroxybutanedioate

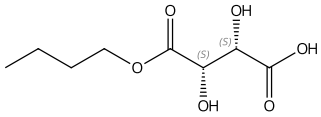
3 References | 1 Reaction | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	206.19	-
Boiling Point (Predicted)	435.7±45.0 °C	Press: 760 Torr
Density (Predicted)	1.334±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.27±0.34	Most Acidic Temp: 25 °C

23

Similarity Score: **88**

1646280-55-8



Absolute stereochemistry shown

$C_8H_{14}O_6$

Butanedioic acid, 2,3-dihydroxy-, 1-butyl ester, (2*S*,3*S*)-

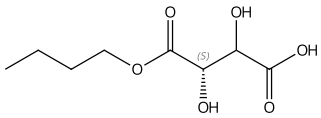
2 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	206.19	-
Boiling Point (Predicted)	435.7±45.0 °C	Press: 760 Torr
Density (Predicted)	1.334±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.27±0.34	Most Acidic Temp: 25 °C

24

Similarity Score: **88**

1194706-78-9



Absolute stereochemistry shown

$C_8H_{14}O_6$

1-Butyl (2*S*)-2,3-dihydroxybutanedioate

1 Reference | 0 Reactions | 0 Suppliers

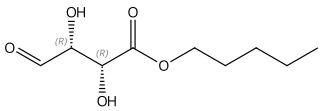
Key Physical Properties	Value	Condition
Molecular Weight	206.19	-
Melting Point (Experimental)	20-25 °C	-
Boiling Point (Experimental)	160-165 °C	Press: 0.5 Torr
Density (Experimental)	1.11 g/cm^3	Temp: 25 °C
pKa (Predicted)	3.27±0.34	Most Acidic Temp: 25 °C

Experimental Properties

25

Similarity Score: **88**

887618-54-4



Relative stereochemistry shown

$C_9H_{16}O_5$

rel-Pentyl (2*R*,3*R*)-2,3-dihydroxy-4-oxobutanoate

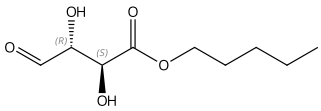
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	204.22	-
Boiling Point (Predicted)	370.9±42.0 °C	Press: 760 Torr
Density (Predicted)	1.175±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.84±0.20	Most Acidic Temp: 25 °C

26

Similarity Score: **88**

887618-43-1



Relative stereochemistry shown

$C_9H_{16}O_5$

rel-Pentyl (2*R*,3*S*)-2,3-dihydroxy-4-oxobutanoate

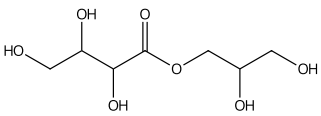
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	204.22	-
Boiling Point (Predicted)	370.9±42.0 °C	Press: 760 Torr
Density (Predicted)	1.175±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.84±0.20	Most Acidic Temp: 25 °C

27

Similarity Score: **87**

1881222-61-2



$C_7H_{14}O_7$

Butanoic acid, 2,3,4-trihydroxy-, 2,3-dihydroxypropyl ester

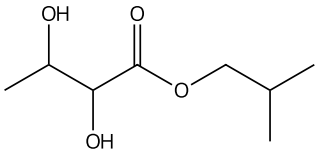
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	210.18	-
Boiling Point (Predicted)	520.1±50.0 °C	Press: 760 Torr
Density (Predicted)	1.542±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.04±0.20	Most Acidic Temp: 25 °C

28

Similarity Score: **86**

158017-59-5



$C_8H_{16}O_4$

Butanoic acid, 2,3-dihydroxy-, 2-methylpropyl ester

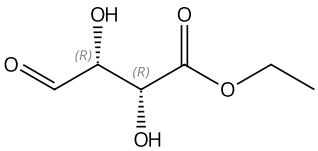
1 Reference | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	176.21	-
Boiling Point (Predicted)	276.8±7.0 °C	Press: 760 Torr
Density (Predicted)	1.099±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.70±0.20	Most Acidic Temp: 25 °C

29

Similarity Score: **86**

887618-50-0



Relative stereochemistry shown

$C_6H_{10}O_5$

rel-Ethyl (2*R*,3*R*)-2,3-dihydroxy-4-oxobutanoate

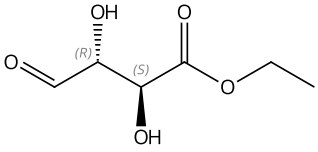
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	162.14	-
Boiling Point (Predicted)	345.5±42.0 °C	Press: 760 Torr
Density (Predicted)	1.306±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.97±0.20	Most Acidic Temp: 25 °C

30

Similarity Score: **86**

887618-39-5



Relative stereochemistry shown

$C_6H_{10}O_5$

rel-Ethyl (2*R*,3*S*)-2,3-dihydroxy-4-oxobutanoate

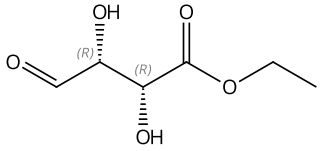
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	162.14	-
Boiling Point (Predicted)	345.5±42.0 °C	Press: 760 Torr
Density (Predicted)	1.306±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.97±0.20	Most Acidic Temp: 25 °C

31

Similarity Score: **86**

885224-03-3



Absolute stereochemistry shown, Rotation (+)

$C_6H_{10}O_5$

Ethyl (2*R*,3*R*)-2,3-dihydroxy-4-oxobutanoate

1 Reference	3 Reactions	2 Suppliers

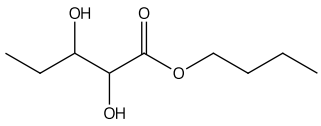
Key Physical Properties	Value	Condition
Molecular Weight	162.14	-
Boiling Point (Predicted)	345.5±42.0 °C	Press: 760 Torr
Density (Predicted)	1.306±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.97±0.20	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

32

Similarity Score: **86**

87826-85-5



$C_9H_{18}O_4$

Pentonic acid, 4,5-dideoxy-, butyl ester

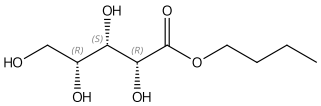
1 Reference	1 Reaction	1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	190.24	-
Boiling Point (Predicted)	299.7±7.0 °C	Press: 760 Torr
Density (Predicted)	1.078±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.50±0.26	Most Acidic Temp: 25 °C

33

Similarity Score: **86**

2283414-15-1



Relative stereochemistry shown

$C_9H_{18}O_6$

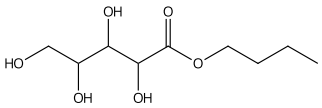
Xylonic acid, butyl ester

2 References	2 Reactions	0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

34 Similarity Score: **86**

887617-99-4



$C_9H_{18}O_6$

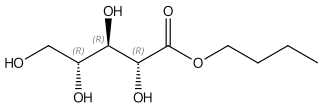
Pentonic acid, butyl ester

1 Reference	0 Reactions	0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

35 Similarity Score: **86**

81105-81-9



Absolute stereochemistry shown

$C_9H_{18}O_6$

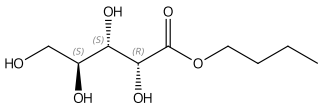
Butyl D-ribonate

1 Reference	0 Reactions	0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

36 Similarity Score: **86**

16751-72-7



Absolute stereochemistry shown

$C_9H_{18}O_6$

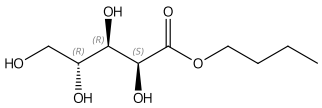
Arabinonic acid, butyl ester, L-

1 Reference	1 Reaction	0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

37 Similarity Score: **86**

16751-71-6



Relative stereochemistry shown

$C_9H_{18}O_6$

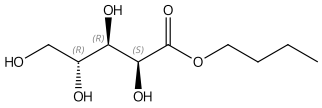
Arabinonic acid, butyl ester, DL-

1 Reference | 1 Reaction | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

38 Similarity Score: **86**

16751-70-5



Absolute stereochemistry shown

$C_9H_{18}O_6$

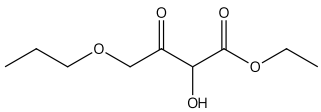
Arabinonic acid, butyl ester, D-

1 Reference | 1 Reaction | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	222.24	-
Boiling Point (Predicted)	423.2±38.0 °C	Press: 760 Torr
Density (Predicted)	1.294±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.11±0.20	Most Acidic Temp: 25 °C

39 Similarity Score: **86**

2296108-69-3



$C_9H_{16}O_5$

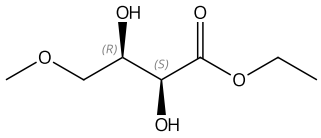
Butanoic acid, 2-hydroxy-3-oxo-4-propoxy-, ethyl ester

0 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	204.22	-
Boiling Point (Predicted)	311.1±27.0 °C	Press: 760 Torr
Density (Predicted)	1.122±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.75±0.20	Most Acidic Temp: 25 °C

40 Similarity Score: **86**

2641824-12-4



Absolute stereochemistry shown

$C_7H_{14}O_5$

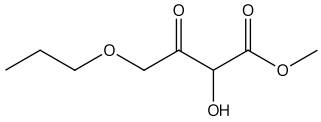
Butanoic acid, 2,3-dihydroxy-4-methoxy-, ethyl ester, (2*S*,3*R*)-

1 Reference | 1 Reaction | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	178.18	-
Boiling Point (Predicted)	280.6±19.0 °C	Press: 760 Torr
Density (Predicted)	1.190±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.29±0.20	Most Acidic Temp: 25 °C

41 Similarity Score: **85**

2300587-91-9



$C_8H_{14}O_5$

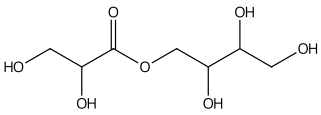
Butanoic acid, 2-hydroxy-3-oxo-4-propoxy-, methyl ester

0 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	190.19	-
Boiling Point (Predicted)	296.1±25.0 °C	Press: 760 Torr
Density (Predicted)	1.149±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.61±0.20	Most Acidic Temp: 25 °C

42 Similarity Score: **85**

1881222-60-1



$C_7H_{14}O_7$

Propanoic acid, 2,3-dihydroxy-, 2,3,4-trihydroxybutyl ester

1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	210.18	-
Boiling Point (Predicted)	522.1±50.0 °C	Press: 760 Torr
Density (Predicted)	1.542±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.15±0.20	Most Acidic Temp: 25 °C