Indexing - Substance

Food and Drug Administration
Indexing - Substance

LINOLEAMIDOPROPYL PG-DIMONIUM CHLORIDE PHOSPHATE (5Q87K461JO)

Alias Name

Name	Name Type	Assigning Territory	Assigning Organization	Reference Document	Citation	Policy
LINOLEAMIDOPROPYL PG-DIMONIUM CHLORIDE PHOSPHATE	primary name					

Substance Information

Mapping	Definition Hash:	dbaeb065-e01e-728b-26ba-c3b56a742dc8

Moiety (mixture component)

Name		Quantity	Undefined not 0

Part1Moiety (mixture component)

Name		Quantity	1

Moiety Characteristics

```
C78H150Cl3N6O10P
  -FDASRS-09071311142D

107103  0  0  0  0  0  0  0  0999 V2000
    3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.1368    0.0000 P   0  0  1  0  0  0  0  0  0  0  0  0
    6.0036   -9.3491    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6886   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3559   -9.3491    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    7.3559   -8.5667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    8.0365   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7084   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2874   -8.6951    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.4964   -8.5446    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3889   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.0697   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.7414   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.4222   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7747   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.4509   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.1228   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.8035   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4797   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1603   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8365   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5085   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4030  -10.3581    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -10.6288    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -11.4195    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.9750  -11.8149    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2901  -11.4196    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.6050  -11.8152    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE

```
  13.9201  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  13.2353  -11.8153    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.5505  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.0941  -10.5337    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   5.2521   -9.9104    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   5.7294   -8.3369    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   6.5382   -8.5225    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.8787   -7.8332    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   6.6576   -7.1879    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   7.7272   -8.0053    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.2310   -7.3866    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   8.7749   -6.6353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   7.9483   -6.6267    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.9868   -7.8199    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.6453   -7.4087    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.3394   -7.7756    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.9980   -7.3646    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
  11.6873   -7.7227    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.3503   -7.3072    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  13.0401   -7.6740    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  13.7028   -7.2629    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  14.4244   -7.5612    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.0641   -7.2143    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.2408   -6.4911    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.0596   -6.0157    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.7533   -6.3825    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.4121   -5.9671    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.3810   -5.1704    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  18.1517   -4.9377    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  18.1837   -4.0902    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  17.5117   -3.6679    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.8101   -4.0387    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  16.1382   -3.6164    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  15.4366   -3.9872    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  14.7647   -3.5649    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.6873   -8.5006    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   4.5892   -8.7303    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.8820   -9.1104    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.8820   -9.8883    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   4.5538  -10.2948    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -10.2684    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -11.0508    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   2.3836  -10.9668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -11.8286    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.2398  -11.5722    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.9118  -11.2231    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   5.5569  -11.6651    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.2644  -11.3248    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   6.9051  -11.7445    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   7.5990  -11.4263    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.2400  -11.8507    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.9384  -11.5281    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.5879  -11.9480    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.2643  -11.5987    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.9050  -12.0452    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.6077  -11.7005    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.2489  -12.1248    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.2423  -12.8959    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.5528  -13.2858    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.5463  -14.0780    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.8568  -14.4683    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.1746  -14.0663    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.4852  -14.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.4785  -15.2483    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.7893  -15.6384    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.7825  -16.4305    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.8522  -12.5181    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   6.9287   -9.1050    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   7.7820   -8.3207    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  11.4236   -8.8659    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.3877   -7.8016    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.9809   -6.8171    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  10.9786   -6.8730    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.3106   -9.6467    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.5437  -10.7867    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.2968  -10.8339    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
 2  3  1  6  0  0  0
 3  4  1  0  0  0  0
 4  5  1  0  0  0  0
 5  6  1  1  0  0  0
 5  7  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 10  1  0  0  0  0
 8 11  1  0  0  0  0
11 12  1  0  0  0  0
12 13  1  0  0  0  0
13 14  1  0  0  0  0
14 15  1  0  0  0  0
15 16  1  0  0  0  0
16 17  1  0  0  0  0
17 18  1  0  0  0  0
18 19  1  0  0  0  0
```

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 19 20  1  0  0  0  0
 20 21  1  0  0  0  0
 21 22  1  0  0  0  0
 22 23  1  0  0  0  0
 23 24  2  0  0  0  0
 24 25  1  0  0  0  0
 25 26  1  0  0  0  0
 26 27  2  0  0  0  0
 27 28  1  0  0  0  0
 28 29  1  0  0  0  0
 29 30  1  0  0  0  0
 30 31  1  0  0  0  0
 31 32  1  0  0  0  0
 15 33  2  0  0  0  0
  2 34  2  0  0  0  0
  2 35  1  0  0  0  0
 35 36  1  0  0  0  0
 36 37  1  0  0  0  0
 37 38  1  1  0  0  0
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 39 40  1  0  0  0  0
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 56 57  1  0  0  0  0
 57 58  1  0  0  0  0
 58 59  2  0  0  0  0
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 61 62  1  0  0  0  0
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 63 64  1  0  0  0  0
 47 65  2  0  0  0  0
  2 66  1  0  0  0  0
 66 67  1  0  0  0  0
 67 68  1  0  0  0  0
 68 69  1  1  0  0  0
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 82 83  1  0  0  0  0
 83 84  1  0  0  0  0
 84 85  1  0  0  0  0
 85 86  1  0  0  0  0
 86 87  2  0  0  0  0
 87 88  1  0  0  0  0
 88 89  1  0  0  0  0
 89 90  2  0  0  0  0
 90 91  1  0  0  0  0
 91 92  1  0  0  0  0
 92 93  1  0  0  0  0
 93 94  1  0  0  0  0
 94 95  1  0  0  0  0
 78 96  2  0  0  0  0
  5 99  1  0  0  0  0
  6100  1  0  0  0  0
 14101  1  0  0  0  0
 37102  1  0  0  0  0
 38103  1  0  0  0  0
 46104  1  0  0  0  0
 68105  1  0  0  0  0
 69106  1  0  0  0  0
 77107  1  0  0  0  0
M  CHG  6   1  -1   8   1  40   1  71   1  97  -1  98  -1
M  STY  1   1 MUL
M  SLB  1   1   1
M  SAL   1  3   1  97  98
M  SPA   1  1   1
M  SMT   1 3
M  SDI   1  4    2.7880  -16.9093    2.7880  -15.4944
M  SDI   1  4    4.4530  -15.4944    4.4530  -16.9093
M  END
```

Chemical Structures, InChI	InChI=1S/C78H147N6O10P.3ClH/c1-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-58-76(88)79-61-55-64-82(4,5)67-73(85)70-92-95(91,93-71-74(86)68-83(6,7)65-56-62-80-77(89)59-53-50-47-44-41-38-35-32-29-26-23-20-17-14-11-2)94-72-75(87)69-84(8,9)66-57-63-81-78(90)60-54-51-48-45-42-39-36-33-30-27-24-21-18-15-12-3;;;/h22-27,31-36,73-75,85-87H,10-21,28-30,37-72H2,1-9H3;3*1H/b25-22-,26-23-,27-24-,34-31-,35-32-,36-33-;;;/t73-,74-,75-;;;/m0.../s1
Chemical Structure, InChIKey	ISRLGZXSKRDKID-HICHISTASA-N

Part2Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

```
C78H150Cl3N6O10P
  -FDASRS-090713111142D

107103  0  0  0  0  0  0  0  0999 V2000
    3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.1368    0.0000 P   0  0  2  0  0  0  0  0  0  0  0  0
    6.0036   -9.3491    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6886   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3559   -9.3491    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    7.3559   -8.5667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    8.0365   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7084   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2874   -8.6951    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.4964   -8.5446    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3889   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.0697   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.7414   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.4222   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7747   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.4509   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.1228   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.8035   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4797   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1603   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8365   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5085   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4030  -10.3581    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -10.6288    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -11.4195    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.9750  -11.8149    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2901  -11.4196    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.6050  -11.8152    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.9201  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2353  -11.8153    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.5505  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941  -10.5337    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.9104    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.7294   -8.3369    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.5382   -8.5225    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.8787   -7.8332    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    6.6576   -7.1879    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    7.7272   -8.0053    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.2310   -7.3866    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    8.7749   -6.6353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9483   -6.6267    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.9868   -7.8199    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.6453   -7.4087    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.3394   -7.7756    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.9980   -7.3646    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.6873   -7.7227    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.3503   -7.3072    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.0401   -7.6740    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.7028   -7.2629    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.4244   -7.5612    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.0641   -7.2143    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2408   -6.4911    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.0596   -6.0157    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.7533   -6.3825    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4121   -5.9671    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.3810   -5.1704    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.1517   -4.9377    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.1837   -4.0902    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5117   -3.6679    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8101   -4.0387    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1382   -3.6164    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4366   -3.9872    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.7647   -3.5649    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.6873   -8.5006    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.5892   -8.7303    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.8820   -9.1104    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8820   -9.8883    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE

```
   4.5538  -10.2948    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -10.2684    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -11.0508    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   2.3836  -10.9668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1836  -11.8286    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.2398  -11.5722    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.9118  -11.2231    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   5.5569  -11.6651    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.2644  -11.3248    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   6.9051  -11.7445    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   7.5990  -11.4263    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.2400  -11.8507    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.9384  -11.5281    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.5879  -11.9480    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.2643  -11.5987    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.9050  -12.0452    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.6077  -11.7005    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.2489  -12.1248    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  12.2423  -12.8959    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.5528  -13.2858    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  11.5463  -14.0780    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.8568  -14.4683    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  10.1746  -14.0663    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.4852  -14.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   9.4785  -15.2483    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.7893  -15.6384    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   8.7825  -16.4305    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.8522  -12.5181    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   6.9287   -9.1050    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   7.7820   -8.3207    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  11.4236   -8.8659    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.3877   -7.8016    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.9809   -6.8171    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  10.9786   -6.8730    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.3106   -9.6467    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.5437  -10.7867    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.2968  -10.8339    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
 2  3  1  0  0  0  0
 3  4  1  0  0  0  0
 4  5  1  0  0  0  0
 5  6  1  0  0  0  0
 5  7  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 10  1  0  0  0  0
 8 11  1  0  0  0  0
11 12  1  0  0  0  0
12 13  1  0  0  0  0
13 14  1  0  0  0  0
14 15  1  0  0  0  0
15 16  1  0  0  0  0
16 17  1  0  0  0  0
17 18  1  0  0  0  0
18 19  1  0  0  0  0
19 20  1  0  0  0  0
20 21  1  0  0  0  0
21 22  1  0  0  0  0
22 23  1  0  0  0  0
23 24  2  0  0  0  0
24 25  1  0  0  0  0
25 26  1  0  0  0  0
26 27  2  0  0  0  0
27 28  1  0  0  0  0
28 29  1  0  0  0  0
29 30  1  0  0  0  0
30 31  1  0  0  0  0
31 32  1  0  0  0  0
15 33  2  0  0  0  0
 2 34  2  6  0  0  0
 2 35  1  0  0  0  0
35 36  1  0  0  0  0
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37 39  1  0  0  0  0
39 40  1  0  0  0  0
40 41  1  0  0  0  0
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46 47  1  0  0  0  0
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48 49  1  0  0  0  0
49 50  1  0  0  0  0
50 51  1  0  0  0  0
51 52  1  0  0  0  0
52 53  1  0  0  0  0
53 54  1  0  0  0  0
54 55  1  0  0  0  0
55 56  2  0  0  0  0
56 57  1  0  0  0  0
57 58  1  0  0  0  0
```

	58 59 2 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0 63 64 1 0 0 0 0 47 65 2 0 0 0 0 2 66 1 0 0 0 0 66 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 68 70 1 0 0 0 0 70 71 1 0 0 0 0 71 72 1 0 0 0 0 71 73 1 0 0 0 0 71 74 1 0 0 0 0 74 75 1 0 0 0 0 75 76 1 0 0 0 0 76 77 1 0 0 0 0 77 78 1 0 0 0 0 78 79 1 0 0 0 0 79 80 1 0 0 0 0 80 81 1 0 0 0 0 81 82 1 0 0 0 0 82 83 1 0 0 0 0 83 84 1 0 0 0 0 84 85 1 0 0 0 0 85 86 1 0 0 0 0 86 87 2 0 0 0 0 87 88 1 0 0 0 0 88 89 1 0 0 0 0 89 90 2 0 0 0 0 90 91 1 0 0 0 0 91 92 1 0 0 0 0 92 93 1 0 0 0 0 93 94 1 0 0 0 0 94 95 1 0 0 0 0 78 96 2 0 0 0 0 5 99 1 1 0 0 0 6100 1 0 0 0 0 14101 1 0 0 0 0 37102 1 1 0 0 0 38103 1 0 0 0 0 46104 1 0 0 0 0 68105 1 1 0 0 0 69106 1 0 0 0 0 77107 1 0 0 0 0 M CHG 6 1 -1 8 1 40 1 71 1 97 -1 98 -1 M STY 1 1 MUL M SLB 1 1 1 M SAL 1 3 1 97 98 M SPA 1 1 1 M SMT 1 3 M SDI 1 4 2.7880 -16.9093 2.7880 -15.4944 M SDI 1 4 4.4530 -15.4944 4.4530 -16.9093 M END
Chemical Structures, InChI	InChI=1S/C78H147N6O10P.3ClH/c1-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-58-76(88)79-61-55-64-82(4,5)67-73(85)70-92-95(91,93-71-74(86)68-83(6,7)65-56-62-80-77(89)59-53-50-47-44-41-38-35-32-29-26-23-20-17-14-11-2)94-72-75(87)69-84(8,9)66-57-63-81-78(90)60-54-51-48-45-42-39-36-33-30-27-24-21-18-15-12-3;;;/h22-27,31-36,73-75,85-87H,10-21,28-30,37-72H2,1-9H3;3*1H/b25-22-,26-23-,27-24-,34-31-,35-32-,36-33-;;;/t73-,74-,75-;;;/m1../s1
Chemical Structure, InChI Key	ISRLGZXSKRDKID-AOTDMZJUSA-N

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Part1Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

	C78H150Cl3N6O10P -FDASRS-09071311142D

```
107103  0  0  0  0  0  0  0  0999 V2000
    3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.1368    0.0000 P   0  0  1  0  0  0  0  0  0  0  0  0
    6.0036   -9.3491    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6886   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3559   -9.3491    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    7.3559   -8.5667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    8.0365   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7084   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2874   -8.6951    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.4964   -8.5446    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3889   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.0697   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.7414   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.4222   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7747   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.4509   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.1228   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.8035   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4797   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1603   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8365   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5085   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4030  -10.3581    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -10.6288    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -11.4195    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.9750  -11.8149    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2901  -11.4196    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.6050  -11.8152    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.9201  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2353  -11.8153    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.5505  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941  -10.5337    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.9104    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.7294   -8.3369    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.5382   -8.5225    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.8787   -7.8332    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
    6.6576   -7.1879    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    7.7272   -8.0053    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.2310   -7.3866    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    8.7749   -6.6353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9483   -6.6267    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.9868   -7.8199    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.6453   -7.4087    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.3394   -7.7756    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.9980   -7.3646    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   11.6873   -7.7227    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.3503   -7.3072    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.0401   -7.6740    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.7028   -7.2629    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.4244   -7.5612    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.0641   -7.2143    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2408   -6.4911    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.0596   -6.0157    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.7533   -6.3825    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4121   -5.9671    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.3810   -5.1704    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.1517   -4.9377    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   18.1837   -4.0902    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5117   -3.6679    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8101   -4.0387    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1382   -3.6164    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4366   -3.9872    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.7647   -3.5649    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.6873   -8.5006    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.5892   -8.7303    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.8820   -9.1104    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8820   -9.8883    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    4.5538  -10.2948    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.1836  -10.2684    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1836  -11.0508    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    2.3836  -10.9668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1836  -11.8286    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.2398  -11.5722    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9118  -11.2231    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5569  -11.6651    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.2644  -11.3248    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    6.9051  -11.7445    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.5990  -11.4263    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.2400  -11.8507    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.9384  -11.5281    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.5879  -11.9480    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.2643  -11.5987    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.9050  -12.0452    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.6077  -11.7005    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2489  -12.1248    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.2423  -12.8959    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.5528  -13.2858    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.5463  -14.0780    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.8568  -14.4683    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.1746  -14.0663    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.4852  -14.4565    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.4785  -15.2483    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7893  -15.6384    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE

```
   8.7825  -16.4305    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   6.8522  -12.5181    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   6.9287   -9.1050    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   7.7820   -8.3207    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  11.4236   -8.8659    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.3877   -7.8016    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.9809   -6.8171    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  10.9786   -6.8730    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.3106   -9.6467    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.5437  -10.7867    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.2968  -10.8339    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
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 5  6  1  0  0  0  0
 5  7  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 10  1  0  0  0  0
 8 11  1  0  0  0  0
11 12  1  0  0  0  0
12 13  1  0  0  0  0
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22 23  1  0  0  0  0
23 24  2  0  0  0  0
24 25  1  0  0  0  0
25 26  1  0  0  0  0
26 27  2  0  0  0  0
27 28  1  0  0  0  0
28 29  1  0  0  0  0
29 30  1  0  0  0  0
30 31  1  0  0  0  0
31 32  1  0  0  0  0
15 33  2  0  0  0  0
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40 42  1  0  0  0  0
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80 81  1  0  0  0  0
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82 83  1  0  0  0  0
83 84  1  0  0  0  0
```

	84 85 1 0 0 0 0 85 86 1 0 0 0 0 86 87 2 0 0 0 0 87 88 1 0 0 0 0 88 89 1 0 0 0 0 89 90 2 0 0 0 0 90 91 1 0 0 0 0 91 92 1 0 0 0 0 92 93 1 0 0 0 0 93 94 1 0 0 0 0 94 95 1 0 0 0 0 78 96 2 0 0 0 0 5 99 1 6 0 0 0 6100 1 0 0 0 0 14101 1 0 0 0 0 37102 1 6 0 0 0 38103 1 0 0 0 0 46104 1 0 0 0 0 68105 1 1 0 0 0 69106 1 0 0 0 0 77107 1 0 0 0 0 M CHG 6 1 -1 8 1 40 1 71 1 97 -1 98 -1 M STY 1 1 MUL M SLB 1 1 1 M SAL 1 3 1 97 98 M SPA 1 1 1 M SMT 1 3 M SDI 1 4 2.7880 -16.9093 2.7880 -15.4944 M SDI 1 4 4.4530 -15.4944 4.4530 -16.9093 M END
Chemical Structures, InChI	InChI=1S/C78H147N6O10P.3ClH/c1-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-58-76(88)79-61-55-64-82(4,5)67-73(85)70-92-95(91,93-71-74(86)68-83(6,7)65-56-62-80-77(89)59-53-50-47-44-41-38-35-32-29-26-23-20-17-14-11-2)94-72-75(87)69-84(8,9)66-57-63-81-78(90)60-54-51-48-45-42-39-36-33-30-27-24-21-18-15-12-3;;;/h22-27,31-36,73-75,85-87H,10-21,28-30,37-72H2,1-9H3;3*1H/b25-22-,26-23-,27-24-,34-31-,35-32-,36-33-;;;/t73-,74-,75+;;;/m0../s1
Chemical Structure, InChI Key	ISRLGZXSKRDKID-QEQZMKTCSA-N

Part2Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

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C78H150Cl3N6O10P
  -FDASRS-09071311142D

107103  0  0  0  0  0  0  0  0999 V2000
    3.4385  -16.2818    0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.1368    0.0000 P   0  0  2  0  0  0  0  0  0  0  0  0
    6.0036   -9.3491    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6886   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3559   -9.3491    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    7.3559   -8.5667    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    8.0365   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7084   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    9.2874   -8.6951    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.4964   -8.5446    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3889   -9.7424    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.0697   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.7414   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.4222   -9.3579    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.7747   -9.3579    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.4509   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.1228   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.8035   -9.7558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.4797   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.1603   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.8365   -9.3668    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.5085   -9.7601    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   17.4030  -10.3581    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -10.6288    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   16.6598  -11.4195    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.9750  -11.8149    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   15.2901  -11.4196    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.6050  -11.8152    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.9201  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2353  -11.8153    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.5505  -11.4197    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.0941  -10.5337    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.2521   -9.9104    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    5.7294   -8.3369    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.5382   -8.5225    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.8787   -7.8332    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
```

	6.6576 -7.1879 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 7.7272 -8.0053 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.2310 -7.3866 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 8.7749 -6.6353 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.9483 -6.6267 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.9868 -7.8199 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.6453 -7.4087 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.3394 -7.7756 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.9980 -7.3646 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 11.6873 -7.7227 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.3503 -7.3072 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.0401 -7.6740 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.7028 -7.2629 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.4244 -7.5612 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.0641 -7.2143 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.2408 -6.4911 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.0596 -6.0157 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.7533 -6.3825 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 17.4121 -5.9671 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 17.3810 -5.1704 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 18.1517 -4.9377 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 18.1837 -4.0902 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 17.5117 -3.6679 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.8101 -4.0387 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 16.1382 -3.6164 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 15.4366 -3.9872 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.7647 -3.5649 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.6873 -8.5006 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 4.5892 -8.7303 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.8820 -9.1104 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.8820 -9.8883 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 4.5538 -10.2948 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.1836 -10.2684 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.1836 -11.0508 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 2.3836 -10.9668 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3.1836 -11.8286 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.2398 -11.5722 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.9118 -11.2231 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5.5569 -11.6651 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.2644 -11.3248 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 6.9051 -11.7445 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.5990 -11.4263 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.2400 -11.8507 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.9384 -11.5281 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.5879 -11.9480 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.2643 -11.5987 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.9050 -12.0452 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.6077 -11.7005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.2489 -12.1248 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.2423 -12.8959 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.5528 -13.2858 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 11.5463 -14.0780 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.8568 -14.4683 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.1746 -14.0663 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.4852 -14.4565 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 9.4785 -15.2483 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.7893 -15.6384 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8.7825 -16.4305 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6.8522 -12.5181 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3.4385 -16.2818 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 3.4385 -16.2818 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6.9287 -9.1050 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 7.7820 -8.3207 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11.4236 -8.8659 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 6.3877 -7.8016 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 6.9809 -6.8171 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 10.9786 -6.8730 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 4.3106 -9.6467 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 4.5437 -10.7867 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 6.2968 -10.8339 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
Chemical Structure, MOLFILE	2 3 1 0 0 0 0 3 4 1 0 0 0 0 4 5 1 0 0 0 0 5 6 1 0 0 0 0 5 7 1 0 0 0 0 7 8 1 0 0 0 0 8 9 1 0 0 0 0 8 10 1 0 0 0 0 8 11 1 0 0 0 0 11 12 1 0 0 0 0 12 13 1 0 0 0 0 13 14 1 0 0 0 0 14 15 1 0 0 0 0 15 16 1 0 0 0 0 16 17 1 0 0 0 0 17 18 1 0 0 0 0 18 19 1 0 0 0 0 19 20 1 0 0 0 0 20 21 1 0 0 0 0 21 22 1 0 0 0 0 22 23 1 0 0 0 0 23 24 2 0 0 0 0 24 25 1 0 0 0 0 25 26 1 0 0 0 0 26 27 2 0 0 0 0

	27 28 1 0 0 0 0 28 29 1 0 0 0 0 29 30 1 0 0 0 0 30 31 1 0 0 0 0 31 32 1 0 0 0 0 15 33 2 0 0 0 0 2 34 2 6 0 0 0 2 35 1 0 0 0 0 35 36 1 0 0 0 0 36 37 1 0 0 0 0 37 38 1 0 0 0 0 37 39 1 0 0 0 0 39 40 1 0 0 0 0 40 41 1 0 0 0 0 40 42 1 0 0 0 0 40 43 1 0 0 0 0 43 44 1 0 0 0 0 44 45 1 0 0 0 0 45 46 1 0 0 0 0 46 47 1 0 0 0 0 47 48 1 0 0 0 0 48 49 1 0 0 0 0 49 50 1 0 0 0 0 50 51 1 0 0 0 0 51 52 1 0 0 0 0 52 53 1 0 0 0 0 53 54 1 0 0 0 0 54 55 1 0 0 0 0 55 56 2 0 0 0 0 56 57 1 0 0 0 0 57 58 1 0 0 0 0 58 59 2 0 0 0 0 59 60 1 0 0 0 0 60 61 1 0 0 0 0 61 62 1 0 0 0 0 62 63 1 0 0 0 0 63 64 1 0 0 0 0 47 65 2 0 0 0 0 2 66 1 0 0 0 0 66 67 1 0 0 0 0 67 68 1 0 0 0 0 68 69 1 0 0 0 0 68 70 1 0 0 0 0 70 71 1 0 0 0 0 71 72 1 0 0 0 0 71 73 1 0 0 0 0 71 74 1 0 0 0 0 74 75 1 0 0 0 0 75 76 1 0 0 0 0 76 77 1 0 0 0 0 77 78 1 0 0 0 0 78 79 1 0 0 0 0 79 80 1 0 0 0 0 80 81 1 0 0 0 0 81 82 1 0 0 0 0 82 83 1 0 0 0 0 83 84 1 0 0 0 0 84 85 1 0 0 0 0 85 86 1 0 0 0 0 86 87 2 0 0 0 0 87 88 1 0 0 0 0 88 89 1 0 0 0 0 89 90 2 0 0 0 0 90 91 1 0 0 0 0 91 92 1 0 0 0 0 92 93 1 0 0 0 0 93 94 1 0 0 0 0 94 95 1 0 0 0 0 78 96 2 0 0 0 0 5 99 1 1 0 0 0 6100 1 0 0 0 0 14101 1 0 0 0 0 37102 1 1 0 0 0 38103 1 0 0 0 0 46104 1 0 0 0 0 68105 1 6 0 0 0 69106 1 0 0 0 0 77107 1 0 0 0 0 M CHG 6 1 -1 8 1 40 1 71 1 97 -1 98 -1 M STY 1 1 MUL M SLB 1 1 1 M SAL 1 3 1 97 98 M SPA 1 1 1 M SMT 1 3 M SDI 1 4 2.7880 -16.9093 2.7880 -15.4944 M SDI 1 4 4.4530 -15.4944 4.4530 -16.9093 M END
Chemical Structures, InChI	InChI=1S/C78H147N6O10P.3ClH/c1-10-13-16-19-22-25-28-31-34-37-40-43-46-49-52-58-76(88)79-61-55-64-82(4,5)67-73(85)70-92-95(91,93-71-74(86)68-83(6,7)65-56-62-80-77(89)59-53-50-47-44-41-38-35-32-29-26-23-20-17-14-11-2)94-72-75(87)69-84(8,9)66-57-63-81-78(90)60-54-51-48-45-42-39-36-33-30-27-24-21-18-15-12-3;;;/h22-27,31-36,73-75,85-87H,10-21,28-30,37-72H2,1-9H3;3*1H/b25-22-,26-23-,27-24-,34-31-,35-32-,36-33-;;;/t73-,74-,75+;;;/m1../s1

Chemical Structure, InChIKey	ISRLGZXSKRDKID-LCMQBHBMSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	**Item Code (Source)**	5Q87K461JO

Labeler - Food and Drug Administration (927645523)

Revised: 9/2013 Food and Drug Administration