Indexing - Substance

Food and Drug Administration
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LUTEIN (X72A60C9MT)

Alias Name

Name	Name Type	Assigning Territory	Assigning Organization	Reference Document	Citation	Policy
LUTEIN	primary name					

Substance Information

Mapping	**Definition Hash:**	3fb0c8d0-439f-8ab4-77ee-986cf2c5b3ea

Moiety

Name		**Quantity**	1

Moiety Characteristics

```
  -FDASRS-09261316272D

 57 58  0  0  1  0  0  0  0  0999 V2000
    1.3670   -3.5020    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8003   -3.9758    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
    0.4313   -4.6162    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3066   -4.6162    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6757   -3.9758    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   -1.4298   -4.0020    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3066   -3.3353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.4313   -3.3353    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8003   -2.6949    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9094   -5.2471    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3054   -5.3459    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.5663   -4.6176    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4748   -5.1297    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.2630   -4.3659    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8297   -4.8396    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5224   -4.5879    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.6525   -3.8624    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.0890   -5.0616    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.7816   -4.8099    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.3482   -5.2837    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.0450   -5.0319    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.1709   -4.3064    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.8069   -5.6739    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.5036   -5.4220    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.0703   -5.8958    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.7628   -5.6441    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3295   -6.1179    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.2036   -6.8475    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   10.0262   -5.8661    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   10.5929   -6.3399    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.2855   -6.0881    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.8522   -6.5619    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.5448   -6.3101    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.1114   -6.7839    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.8082   -6.5321    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.3748   -7.0101    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

Chemical Structure, MOLFILE	14.2447 -7.7356 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 14.7498 -8.2152 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 13.5522 -7.9873 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.9855 -7.5135 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.2887 -7.7653 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 13.6330 -5.8918 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 14.3748 -6.0584 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 12.6749 -5.5847 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11.7221 -7.2915 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11.4157 -5.3585 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10.4628 -7.0695 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 10.1523 -5.1364 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 8.8930 -4.9145 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7.9401 -6.6255 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 7.6295 -4.6924 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 6.6809 -6.4035 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 5.2223 -6.0134 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4.9117 -4.0844 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 3.9589 -5.7913 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 2.6996 -5.5693 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2.3891 -3.6363 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 2 1 1 1 0 0 0 2 3 1 0 0 0 0 4 3 1 0 0 0 0 4 5 1 0 0 0 0 5 6 1 1 0 0 0 7 5 1 0 0 0 0 7 8 2 0 0 0 0 8 2 1 0 0 0 0 9 8 1 0 0 0 0 10 3 1 0 0 0 0 11 3 1 0 0 0 0 12 2 1 0 0 0 0 12 13 1 0 0 0 0 14 12 2 0 0 0 0 14 15 1 0 0 0 0 16 15 2 0 0 0 0 16 17 1 0 0 0 0 18 16 1 0 0 0 0 18 19 2 0 0 0 0 19 20 1 0 0 0 0 21 20 2 0 0 0 0 21 22 1 0 0 0 0 23 21 1 0 0 0 0 23 24 2 0 0 0 0 24 25 1 0 0 0 0 25 26 2 0 0 0 0 27 26 1 0 0 0 0 27 28 1 0 0 0 0 29 27 2 0 0 0 0 29 30 1 0 0 0 0 30 31 2 0 0 0 0 32 31 1 0 0 0 0 32 33 2 0 0 0 0 33 34 1 0 0 0 0 34 35 1 0 0 0 0 36 35 1 0 0 0 0 36 37 1 0 0 0 0 37 38 1 6 0 0 0 39 37 1 0 0 0 0 39 40 1 0 0 0 0 40 34 2 0 0 0 0 41 40 1 0 0 0 0 42 35 1 0 0 0 0 43 35 1 0 0 0 0 33 44 1 0 0 0 0 32 45 1 0 0 0 0 46 31 1 0 0 0 0 30 47 1 0 0 0 0 29 48 1 0 0 0 0 49 26 1 0 0 0 0 25 50 1 0 0 0 0 24 51 1 0 0 0 0 23 52 1 0 0 0 0 53 20 1 0 0 0 0 19 54 1 0 0 0 0 18 55 1 0 0 0 0 56 15 1 0 0 0 0 14 57 1 0 0 0 0

	M END
Chemical Structures, InChI	InChI=1S/C40H56O2/c1-29(17-13-19-31(3)21-23-37-33(5)25-35(41)27-39(37,7)8)15-11-12-16-30(2)18-14-20-32(4)22-24-38-34(6)26-36(42)28-40(38,9)10/h11-25,35-37,41-42H,26-28H2,1-10H3/b12-11+,17-13+,18-14+,23-21+,24-22+,29-15+,30-16+,31-19+,32-20+/t35-,36+,37-/m0/s1
Chemical Structure, InChI Key	KBPHJBAIARWVSC-RGZFRNHPSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	**Item Code (Source)**	X72A60C9MT

Labeler - Food and Drug Administration (927645523)

Revised: 9/2013 Food and Drug Administration