Indexing - Substance

Food and Drug Administration
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ACETYLCARNITINE, (+/-)- (07OP6H4V4A)

Alias Name

Name	Name Type	Assigning Territory	Assigning Organization	Reference Document	Citation	Policy
ACETYLCARNITINE, (+/-)-	primary name					

Substance Information

Mapping	**Definition Hash:**	9f2b3229-7800-56bb-e3d3-c9e0bae1cf53

Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

Chemical Structure, MOLFILE

```
C9H17NO4
  -FDASRS-09061311012D

 15 14  0  0  0  0  0  0  0  0999 V2000
   13.9901   -8.2761    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.7026   -7.8636    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2776   -7.8719    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   11.8526   -7.8761    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   13.2651   -6.2219    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2776   -7.0469    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   15.4151   -8.2761    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   14.7026   -7.0386    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   12.5526   -5.8094    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   12.5651   -8.2844    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.1401   -8.2886    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.8526   -7.0511    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.1359   -7.4636    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.9776   -5.8052    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.8351   -7.6168    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  4 10  1  0  0  0  0
  5  6  1  0  0  0  0
  3  6  1  6  0  0  0
  2  7  1  0  0  0  0
  2  8  2  0  0  0  0
  5  9  2  0  0  0  0
  3 10  1  0  0  0  0
  4 11  1  0  0  0  0
  4 12  1  0  0  0  0
  4 13  1  0  0  0  0
  5 14  1  0  0  0  0
  3 15  1  0  0  0  0
M  CHG  2   4   1   7  -1
M  END
```

Chemical Structures, InChI	InChI=1S/C9H17NO4/c1-7(11)14-8(5-9(12)13)6-10(2,3)4/h8H,5-6H2,1-4H3/t8-/m1/s1
Chemical Structure, InChI Key	RDHQFKQIGNGIED-MRVPVSSYSA-N

Moiety (mixture component)

Name		Quantity	1

Moiety Characteristics

Chemical Structure, MOLFILE

```
C9H17NO4
  -FDASRS-09061311012D

 15 14  0  0  0  0  0  0  0  0999 V2000
   13.9901   -8.2761    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   14.7026   -7.8636    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2776   -7.8719    0.0000 C   0  0  2  0  0  0  0  0  0  0  0  0
   11.8526   -7.8761    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   13.2651   -6.2219    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.2776   -7.0469    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   15.4151   -8.2761    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   14.7026   -7.0386    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   12.5526   -5.8094    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   12.5651   -8.2844    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.1401   -8.2886    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.8526   -7.0511    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   11.1359   -7.4636    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   13.9776   -5.8052    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   12.8351   -7.6168    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  4 10  1  0  0  0  0
  5  6  1  0  0  0  0
  3  6  1  0  0  0  0
  2  7  1  0  0  0  0
  2  8  2  0  0  0  0
  5  9  2  0  0  0  0
  3 10  1  0  0  0  0
  4 11  1  0  0  0  0
  4 12  1  0  0  0  0
  4 13  1  0  0  0  0
  5 14  1  0  0  0  0
  3 15  1  6  0  0  0
M  CHG  2   4   1   7  -1
M  END
```

Chemical Structures, InChI	InChI=1S/C9H17NO4/c1-7(11)14-8(5-9(12)13)6-10(2,3)4/h8H,5-6H2,1-4H3/t8-/m0/s1
Chemical Structure, InChI Key	RDHQFKQIGNGIED-QMMMGPOBSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	Item Code (Source)	07OP6H4V4A

Labeler - Food and Drug Administration (927645523)