Indexing - Substance

Food and Drug Administration
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METHOHEXITAL (E5B8ND5IPE)

Alias Name

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

Substance Information

Mapping	**Definition Hash:**	bbd36012-510e-255c-abf6-62dce94bffef

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Part1Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

Chemical Structure, MOLFILE

```
C14H18N2O3
  -FDASRS-01291411012D

 21 21  0  0  0  0  0  0  0  0999 V2000
   -4.3208   -4.6792    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6083   -4.2750    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.0375   -4.2750    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6083   -3.4417    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   -5.0375   -3.4417    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3208   -3.0375    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3708   -2.7292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5458   -2.7292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8958   -4.6917    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1958   -2.7292    0.0000 C   0  0  1  0  0  0  0  0  0  0  0  0
   -5.7583   -4.6875    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3208   -2.2125    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7833   -3.4417    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3208   -5.5042    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3708   -4.1542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5458   -4.1542    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7208   -2.7292    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.2000   -1.9042    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3125   -2.0125    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4793   -3.1837    0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6902   -2.5977    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
  2  4  1  0  0  0  0
  3  5  1  0  0  0  0
  4  6  1  0  0  0  0
  7 10  1  0  0  0  0
  7  8  3  0  0  0  0
  2  9  2  0  0  0  0
  4 10  1  0  0  0  0
  3 11  2  0  0  0  0
  6 12  2  0  0  0  0
  4 13  1  6  0  0  0
```

	1 14 1 0 0 0 0 13 15 1 0 0 0 0 15 16 2 0 0 0 0 8 17 1 0 0 0 0 10 18 1 6 0 0 0 17 19 1 0 0 0 0 5 6 1 0 0 0 0 5 20 1 0 0 0 0 10 21 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C14H18N2O3/c1-5-7-8-10(3)14(9-6-2)11(17)15-13(19)16(4)12(14)18/h6,10H,2,5,9H2,1,3-4H3,(H,15,17,19)/t10-,14-/m1/s1
Chemical Structure, InChIKey	NZXKDOXHBHYTKP-QMTHXVAHSA-N

Part2Moiety (mixture component)

Name		**Quantity**	1

Moiety Characteristics

Chemical Structure, MOLFILE	C14H18N2O3 -FDASRS-01291411012D 21 21 0 0 0 0 0 0 0 0999 V2000 -4.3208 -4.6792 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.0375 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -3.4417 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 -5.0375 -3.4417 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -3.0375 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.3708 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.5458 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.8958 -4.6917 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -3.1958 -2.7292 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 -5.7583 -4.6875 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -2.2125 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -2.7833 -3.4417 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -5.5042 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.3708 -4.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.5458 -4.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.7208 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.2000 -1.9042 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.3125 -2.0125 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.4793 -3.1837 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 -3.6902 -2.5977 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 2 4 1 0 0 0 0 3 5 1 0 0 0 0 4 6 1 0 0 0 0 7 10 1 0 0 0 0 7 8 3 0 0 0 0 2 9 2 0 0 0 0 4 10 1 0 0 0 0 3 11 2 0 0 0 0 6 12 2 0 0 0 0 4 13 1 1 0 0 0 1 14 1 0 0 0 0 13 15 1 0 0 0 0 15 16 2 0 0 0 0 8 17 1 0 0 0 0 10 18 1 1 0 0 0 17 19 1 0 0 0 0 5 6 1 0 0 0 0 5 20 1 0 0 0 0 10 21 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C14H18N2O3/c1-5-7-8-10(3)14(9-6-2)11(17)15-13(19)16(4)12(14)18/h6,10H,2,5,9H2,1,3-4H3,(H,15,17,19)/t10-,14-/m0/s1
Chemical Structure, InChIKey	NZXKDOXHBHYTKP-HZMBPMFUSA-N

Moiety (mixture component)

Name		**Quantity**	Undefined not 0

Part1Moiety (mixture component)

Name		Quantity	1

Moiety Characteristics

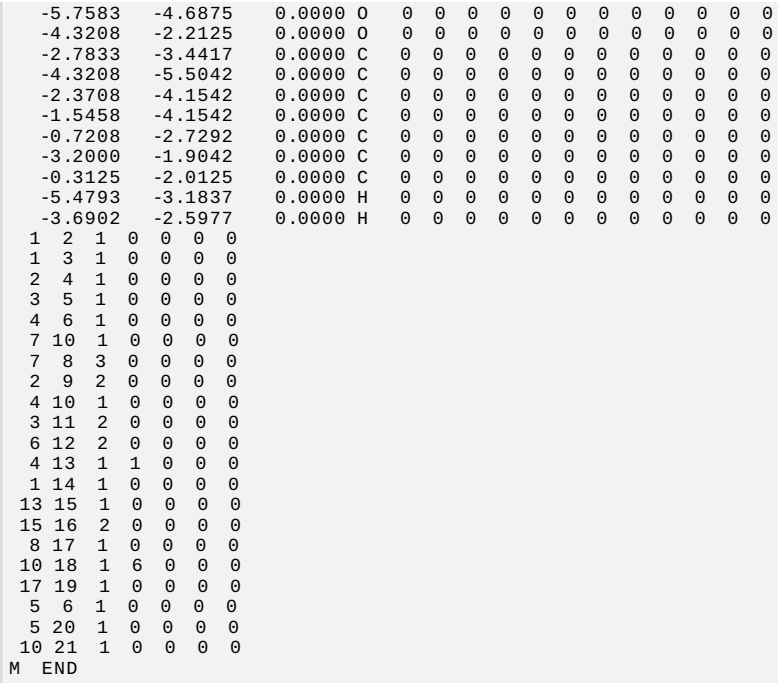
Chemical Structure, MOLFILE	C14H18N2O3 -FDASRS-01291411012D 21 21 0 0 0 0 0 0 0 0999 V2000 -4.3208 -4.6792 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.0375 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -3.4417 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 -5.0375 -3.4417 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -3.0375 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.3708 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.5458 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.8958 -4.6917 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -3.1958 -2.7292 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 -5.7583 -4.6875 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -2.2125 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -2.7833 -3.4417 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -5.5042 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.3708 -4.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.5458 -4.1542 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.7208 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.2000 -1.9042 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -0.3125 -2.0125 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.4793 -3.1837 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 -3.6902 -2.5977 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 2 4 1 0 0 0 0 3 5 1 0 0 0 0 4 6 1 0 0 0 0 7 10 1 0 0 0 0 7 8 3 0 0 0 0 2 9 2 0 0 0 0 4 10 1 0 0 0 0 3 11 2 0 0 0 0 6 12 2 0 0 0 0 4 13 1 6 0 0 0 1 14 1 0 0 0 0 13 15 1 0 0 0 0 15 16 2 0 0 0 0 8 17 1 0 0 0 0 10 18 1 1 0 0 0 17 19 1 0 0 0 0 5 6 1 0 0 0 0 5 20 1 0 0 0 0 10 21 1 0 0 0 0 M END
Chemical Structures, InChI	InChI=1S/C14H18N2O3/c1-5-7-8-10(3)14(9-6-2)11(17)15-13(19)16(4)12(14)18/h6,10H,2,5,9H2,1,3-4H3,(H,15,17,19)/t10-,14+/m0/s1
Chemical Structure, InChIKey	NZXKDOXHBHYTKP-IINYFYTJSA-N

Part2Moiety (mixture component)

Name		Quantity	1

Moiety Characteristics

	C14H18N2O3 -FDASRS-01291411012D 21 21 0 0 0 0 0 0 0 0999 V2000 -4.3208 -4.6792 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -5.0375 -4.2750 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -3.6083 -3.4417 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 -5.0375 -3.4417 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 -4.3208 -3.0375 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.3708 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -1.5458 -2.7292 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 -2.8958 -4.6917 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 -3.1958 -2.7292 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0

Chemical Structure, MOLFILE	
Chemical Structures, InChI	InChI=1S/C14H18N2O3/c1-5-7-8-10(3)14(9-6-2)11(17)15-13(19)16(4)12(14)18/h6,10H,2,5,9H2,1,3-4H3,(H,15,17,19)/t10-,14+/m1/s1
Chemical Structure, InChIKey	NZXKDOXHBHYTKP-YGRLFVJLSA-N

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	**Item Code (Source)**	E5B8ND5IPE

Labeler - Food and Drug Administration (927645523)

Revised: 1/2014 Food and Drug Administration