
[illegible]

7.9375	0.2208	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
8.6500	-0.1875	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0
7.9333	1.0500	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.5208	0.1917	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.2375	-0.2167	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.8042	-0.2208	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-2.0917	0.1917	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-1.3750	-0.2167	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-0.6583	0.1958	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.0583	-0.2125	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
0.7750	0.2000	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
1.4917	-0.2083	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.2083	0.2042	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
2.9208	-0.2042	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
3.6375	0.2083	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
4.3542	-0.2000	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
5.0708	0.2125	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
5.7875	-0.1958	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
6.5042	0.2167	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
7.2208	-0.1917	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
7.9375	0.2208	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
8.6500	-0.1875	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0
7.9333	1.0500	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0
-3.5208	0.1917	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
-4.2375	-0.2167	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	1	0	0	0	0										
14	15	1	0	0	0	0										
15	16	1	0	0	0	0										
23	24	1	0	0	0	0										
37	38	1	0	0	0	0										
28	29	1	0	0	0	0										
37	39	2	0	0	0	0										
22	40	1	0	0	0	0										
29	30	1	0	0	0	0										
40	41	1	0	0	0	0										
24	25	1	0	0	0	0										
30	31	1	0	0	0	0										
31	32	1	0	0	0											

	55 56 1 0 0 0 0
	47 48 1 0 0 0 0
	56 57 1 0 0 0 0
M	CHG 4 1 3 18 -1 38 -1 58 -1
M	STY 1 1 MUL
M	SLB 1 1 1
M	SAL 1 8 17 18 19 20 21 22 23 24
M	SAL 1 8 25 26 27 28 29 30 31 32
M	SAL 1 8 33 34 35 36 37 38 39 40
M	SAL 1 8 41 42 43 44 45 46 47 48
M	SAL 1 8 49 50 51 52 53 54 55 56
M	SAL 1 5 57 58 59 60 61
M	SPA 1 8 2 3 4 5 6 7 8 9
M	SPA 1 8 10 11 12 13 14 15 16 17
M	SPA 1 4 18 19 20 21
M	SMT 1 3
M	SDI 1 4 -5.2500 -0.9000 -5.2500 1.5500
M	SDI 1 4 9.3500 1.5500 9.3500 -0.9000
M	END
Chemical Structures, InChI	InChI=1S/3C18H36O2.Al/c3*1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20;/h3*2-17H2,1H3,(H,19,20);/q;;;+3/p-3
Chemical Structure, InChI Key	CEGOLXSJUTHNZ-UHFFFAOYSA-K

Molecular Bond Types

Product Information

Product Type	INDEXING - SUBSTANCE	Item Code (Source)	U6XF9NP8HM
--------------	----------------------	--------------------	------------

Labeler - Food and Drug Administration (927645523)