

818

počet vazeb

13 13 0 0 0 0 0 0 0999 V2000

počet atomů

4.5981	1.3450	0.0000	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6.3301	0.3450	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2.8660	0.3450	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5.4641	-0.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3.7321	-0.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.5981	0.3450	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5.4641	-1.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3.7321	-1.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7.1962	-0.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6.3301	1.3450	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2.0000	-0.1550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2.8660	1.3450	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4.5981	-1.6550	0.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

značka atomu

souřadnice atomů

1	6	1	0	0	0	0
2	4	1	0	0	0	0
2	9	1	0	0	0	0
2	10	1	0	0	0	0
3	5	1	0	0	0	0
3	11	1	0	0	0	0
3	12	1	0	0	0	0
4	6	2	0	0	0	0
4	7	1	0	0	0	0
5	6	1	0	0	0	0
5	8	2	0	0	0	0
7	13	2	0	0	0	0
8	13	1	0	0	0	0

dvojná vazby mezi atomy 4 a 6

M END

> <DRUGBANK_ID>

DB00818

> <DRUGBANK_GENERIC_NAME>

Propofol

> <DRUGBANK_MOLECULAR_FORMULA>

C12H18O

> <DRUGBANK_MOLECULAR_WEIGHT>

178.2707

