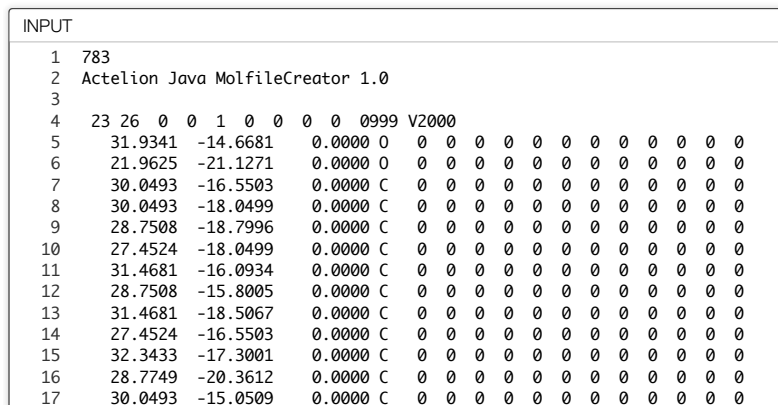
































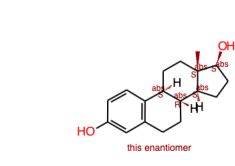


[OpenBabel](#) allows to convert nearly all the chemical formats and it very practical to quickly move from one program to another. On this page we have setup a webservice allowing you to use OpenBabel without having to install it.










HO

this enantiomer

Options	
Input format*	
mol -- MDL MOL format	▼
Output format*	
pdb -- Protein Data Bank format	▼
Generate coordinates	3D ▼
<i>Allows to generate 2D or 3D coordinates</i>	
Add / Delete hydrogens	Add ▼
pH to add hydrogens	7
<i>Specify a pH at which the molecule should be protonated</i>	

Convert

How to proceed ?

1. Enter an input value, for example a SMILES like "CCCC"
2. Select the "Input format", for example "smi"
3. Select an output format, for example "mol"
4. Click on "Convert"

OUTPUT									
1	COMPND	783							
2	AUTHOR	GENERATED BY OPEN BABEL 3.1.1							
3	HETATM	1	O	UNL	1	-5.048	1.118	-0.305	1.00
4	HETATM	2	O	UNL	1	5.795	0.198	-0.543	1.00
5	HETATM	3	C	UNL	1	-2.649	0.542	-0.116	1.00
6	HETATM	4	C	UNL	1	-1.992	-0.774	0.347	1.00
7	HETATM	5	C	UNL	1	-0.502	-0.839	-0.002	1.00
8	HETATM	6	C	UNL	1	0.233	0.357	0.679	1.00
9	HETATM	7	C	UNL	1	-4.102	0.269	0.316	1.00
10	HETATM	8	C	UNL	1	-1.975	1.697	0.630	1.00
11	HETATM	9	C	UNL	1	-2.938	-1.842	-0.198	1.00
12	HETATM	10	C	UNL	1	-0.460	1.712	0.385	1.00
13	HETATM	11	C	UNL	1	-4.335	-1.203	-0.070	1.00
14	HETATM	12	C	UNL	1	0.154	-2.140	0.474	1.00
15	HETATM	13	C	UNL	1	-2.576	0.799	-1.643	1.00
16	HETATM	14	C	UNL	1	1.722	0.327	0.350	1.00
17	HETATM	15	C	UNL	1	1.616	-2.212	0.031	1.00
18	HETATM	16	C	UNL	1	2.363	-0.898	0.071	1.00
19	HETATM	17	C	UNL	1	2.502	1.500	0.372	1.00
20	HETATM	18	C	UNL	1	3.735	-0.912	-0.231	1.00
21	HETATM	19	C	UNL	1	3.864	1.475	0.075	1.00
22	HETATM	20	C	UNL	1	4.471	0.267	-0.233	1.00
23	HETATM	21	H	UNL	1	-2.064	-0.835	1.446	1.00
24	HETATM	22	H	UNL	1	-0.378	-0.782	-1.091	1.00
25	HETATM	23	H	UNL	1	0.172	0.211	1.768	1.00
26	HETATM	24	H	UNL	1	-4.834	2.031	-0.051	1.00
27	HETATM	25	H	UNL	1	6.162	1.098	-0.525	1.00
28	HETATM	26	H	UNL	1	-4.216	0.378	1.402	1.00
29	HETATM	27	H	UNL	1	-2.151	1.602	1.709	1.00
30	HETATM	28	H	UNL	1	-2.407	2.660	0.331	1.00
31	HETATM	29	H	UNL	1	-2.876	-2.778	0.366	1.00
32	HETATM	30	H	UNL	1	-2.721	-2.073	-1.247	1.00
33	HETATM	31	H	UNL	1	0.251	2.032	0.646	1.00

```
Log
=====
*** Open Babel Warning in DoTransformations
    Both -p and -h options are set. All implicit hydr
1 molecule converted
```

