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# 5α-Cholestane

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**Key indicators**

Single-crystal X-ray study
*T* = 120 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.062
*wR* factor = 0.137
Data-to-parameter ratio = 18.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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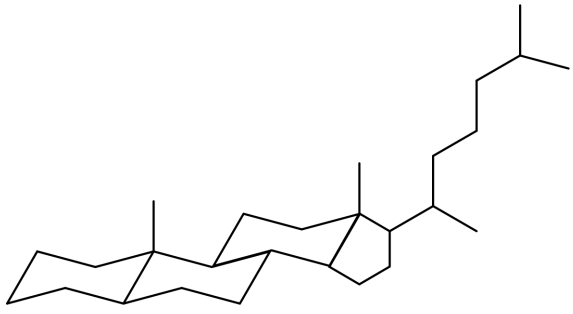
The title compound, $C_{27}H_{48}$, is a steroid derivative composed of a saturated-carbon fused-ring framework with two methyl substituents and an alkyl side chain.

## Comment

The title compound, (I), is a cholesterol steroid-based structure and hence the atom-numbering scheme normally assigned to such structures is employed (Hsu & Nordman, 1983). Cholestane appears in the Cambridge Crystallographic Database (Allen & Kennard, 1993) as entry ZZZKGI (Haner & Norton, 1966); however, there are no deposited coordinates and merely the unit-cell parameters are presented; determination of the structure was therefore deemed worthwhile.



(I)

Cholestane crystallizes with two molecules in the asymmetric unit (Fig. 1). The structure is composed of four fused carbon rings with two methyl substituents, and an alkyl side chain. The three six-membered rings are all in the chair conformation whilst, according to puckering analysis (Cremer & Pople, 1975), the five-membered ring is in a twist conformation about the C13—C14 bond. There are eight chiral centres in the molecule, but the absolute configuration of these sites cannot be assigned with confidence as the absolute structure cannot be determined reliably from this experiment. From the structure presented, these sites exhibit the following chirality: C5 = *R*, C8 = *R*, C9 = *S*, C10 = *S*, C13 = *R*, C14 = *S*, C17 = *R* and C20 = *R*; however, an inversion of the absolute configuration would reverse all these chirality assignments. As a result of the lack of acceptor atoms, there are no classical hydrogen bonds in the crystal structure. The molecules pack as corrugated sheets perpendicular to the *c* axis.

## Experimental

5α-Cholestane was purchased from Aldrich and recrystallized from ethanol/diethyl ether (50:50) in order to produce suitable single crystals.

*Crystal data*

| | |
|---|---|
| $C_{27}H_{48}$ | $D_x$ = 1.055 Mg m$^{-3}$ |
| $M_r$ = 372.65 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1$ | Cell parameters from 6151 reflections |
| $a$ = 11.3936 (3) Å | $\theta$ = 2.9–27.5° |
| $b$ = 10.8972 (3) Å | $\mu$ = 0.06 mm$^{-1}$ |
| $c$ = 19.5047 (7) Å | $T$ = 120 (2) K |
| $\beta$ = 104.2390 (11)° | Plate, colourless |
| $V$ = 2347.27 (12) Å$^3$ | 0.40 × 0.35 × 0.04 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD diffractometer | 5989 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int}$ = 0.076 |
| Absorption correction: multi-scan (*SORTAV*; Blessing, 1997) | $\theta_{max}$ = 27.5° |
| $T_{min}$ = 0.977, $T_{max}$ = 0.998 | $h = -14 \rightarrow 14$ |
| 15024 measured reflections | $k = -14 \rightarrow 11$ |
| 9278 independent reflections | $l = -25 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0563P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.062 | $(\Delta/\sigma)_{max}$ = 0.025 |
| $wR(F^2)$ = 0.137 | $\Delta\rho_{max}$ = 0.63 e Å$^{-3}$ |
| $S$ = 0.99 | $\Delta\rho_{min}$ = −0.62 e Å$^{-3}$ |
| 9278 reflections | Extinction correction: *SHELXL* |
| 498 parameters | Extinction coefficient: 0.047 (2) |
| H-atom parameters constrained | |

All C atoms were refined anisotropically, whilst H atoms were placed in idealized positions and were refined with a riding model. Methyl H atoms were refined as rigid groups allowed to rotate but not tip. The structure crystallizes in the chiral space group $P2_1$ but the absolute structure parameter (Flack, 1983) could not be refined to an acceptable value as the structure is composed purely of C and H atoms.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990).

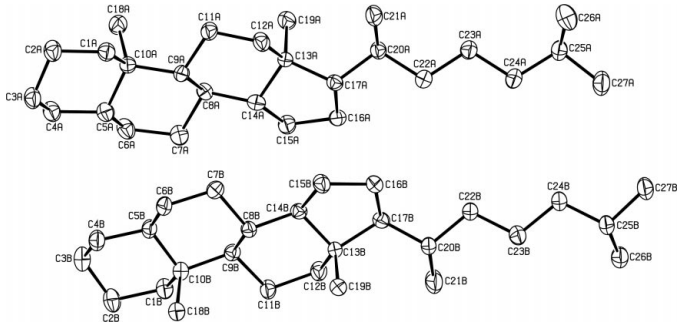



**Figure 1**
View of the two molecules of (I) in the asymmetric unit, with 50% probability displacement ellipsoids.

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