1-(Methoxymethyl)pyrene

The title compound, C₁₈H₁₄O, crystallizes with aromatic π–π stacking interactions.

Comment

With their particular electronic, optical and geometric properties, pyrene and its derivatives (Garcia-Cruz et al., 2004; Takahashi et al., 2004; Borisevich et al., 1992) have attracted considerable recent interest. This is demonstrated in a great number of applications including host–guest (Vögtle, 1996) and metal coordination chemistry (Arrais et al., 2004), as well as fluorescent sensor development (Bren, 2001). Although pyrenes with a functional side arm are important building blocks in this respect, reports on corresponding crystal structures are limited (Foss & Stevens, 1985; Olszak et al., 1989). Here, we describe the structure of 1-(methoxymethyl)pyrene, (I), a new example of this type of compound.

The pyrene part of the molecule shows no significant deviations of bond lengths and angles compared with those of the unsubstituted analogue (Cameron & Trotter, 1965; Allmann, 1970; Hazell et al., 1972; Kai et al., 1978), and is almost planar. The largest deviation from the mean plane through the carbon framework of the pyrene unit is 0.042 (1) Å for atom C1. The torsion angle C2—C1—C17—O1 is 15.1 (1)°, indicating that the methoxymethyl group is turned away from the aromatic plane, while the C—C—O—C fragment itself exhibits a nearly ideal anti-periplanar conformation [179.7 (1)°].

Due to the aromatic nature of the molecule, the crystal packing of (I) is dominated by arene–arene supramolecular contacts. In contrast to the unsubstituted pyrene, which forms face-to-face dimers packed in a herringbone fashion, the crystal structure of (I) is characterized by molecular stacks which are stabilized by offset face-to-face interactions. Within the stacks, the mean distance between consecutive molecules is 3.5 Å. The molecules of neighboring stacks are inclined to each other at an angle of 86.47 (3)°. Hence the compound has an overall packing structure resembling the pattern found in...
the solid state structures of many aromatic compounds (Desiraju, 1989).

**Experimental**

The title compound, (I), was synthesized from commercially available pyrene-1-carbaldehyde, which was initially reduced with sodium borohydride in boiling methanol, following an analogous procedure described for the reduction of anthracene-9-carbaldehyde (Steward, 1960), to yield the intermediate compound 1-(hydroxymethyl)pyrene. This was transformed into 1-(bromomethyl)pyrene by the usual bromination with phosphorus tribromide in chloroform (Okamoto et al., 1990). Subsequent treatment with boiling methanol and recrystallization of the product from the same solvent yielded 60% of compound (I) as colorless needles (m.p. 322–323 K). 1HN M R

**Crystal data**

\[ C_{18}H_{14}O \]

\[ M_r = 246.29 \]

Monoclinic, \( P2_1/n \)

\( a = 4.7220 \) (10) Å

\( b = 20.087 \) (4) Å

\( c = 12.824 \) (3) Å

\( \beta = 91.13 \) (3)

\( V = 1216.1 \) (5) Å³

\[ Z = 4 \]

\[ D_\text{c} = 1.345 \text{ Mg m}^{-3} \]

Mo Kα radiation

\[ \mu = 0.08 \text{ mm}^{-1} \]

\( T = 93 \) (2) K

Prism, colorless

0.41 × 0.20 × 0.17 mm

**Data collection**

Bruker SMART CCD area-detector diffractometer

\( \varphi \) and \( \omega \) scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2000)

19573 measured reflections

3712 independent reflections

2920 reflections with \( I > 2\sigma(I) \)

\( \theta_{\text{max}} = 30.5^\circ \)

**Refinement**

Reﬁnement on \( F^2 \)

\[ wR(F^2) = 0.046 \]

\[ S = 0.97 \]

3712 reflections

172 parameters

H-atom parameters constrained

\[ w = 1/[\sigma^2(F_o^2) + (0.0988P)^2] \]

where \( P = (F_o^2 + 2F_c^2)/3 \)

\( \Delta F_{\text{max}} = 0.48 \) e Å⁻³

\( \Delta F_{\text{min}} = -0.20 \) e Å⁻³

**Figure 1**

Perspective view of (I), showing 50% probability displacement ellipsoids for the non-H atoms.

**Figure 2**

 Packing diagram of (I), viewed down the c axis. H atoms have been omitted.


References


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