Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3,5-Tris(2-isopropylphenoxymethyl)benzene

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.141
Data-to-parameter ratio = 14.8

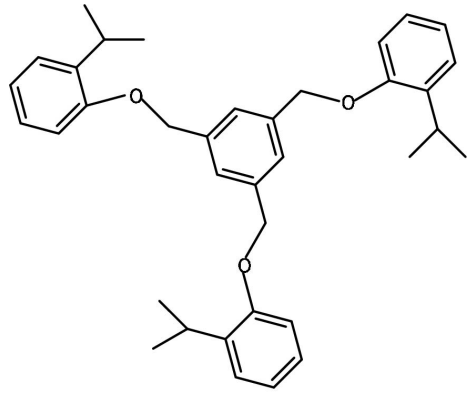
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 31 March 2005
Accepted 5 May 2005
Online 14 May 2005

The title compound, $C_{36}H_{42}O_3$, consists of three 2-isopropylphenoxymethyl groups bonded to the central benzene ring at the 1-, 3- and 5-positions. Intramolecular C—H···O hydrogen bonds seem to have an effect on the molecular conformation.

Comment

The title compound, (I), contains three phenoxymethyl groups which can increase oral absorption. Phenoxymethyl has also been added to penicillin to increase its absorption in oral medicine (Ito *et al.*, 2000; Miko *et al.*, 2004).



(I)

The title molecule, (I), is a phenyl ether derivative, which was synthesized by treating 2-isopropylphenol with 1,3,5-tris(bromomethyl)benzene in dimethylformamide using K_2CO_3 as the base. Since phenyl ethers have been used as antimicrobial agents and hygeine products, they are incorporated into many types of cosmetic formulations (Russell, 2004; Parfitt, 1999).

Some tetra-, tri- and disubstituted methylbenzene derivatives are used for the syntheses of polymers and dentritic molecules (Newkome *et al.*, 1996). In recent years, these polymers have attracted great interest due to their unique properties and important applications (Kuriyama & Otsu, 1984; Kwon *et al.*, 2003).

The intramolecular C—H···O hydrogen bonds (Table 2) seem to be effective on the molecular conformation (Fig. 1). The dihedral angles between rings *A* (C1–C6), *B* (C10–C15), *C* (C19–C24) and *D* (C28–C33) are *A*/*B* 10.7 (7)°, *A*/*C* 66.6 (7)° and *A*/*D* 2.8 (6)°.

Experimental

2-Isopropylphenol (1.20 g, 8.81 mmol) and K_2CO_3 (1.50 g, 10.87 mmol) in dry dimethylformamide (40 ml) were heated and

stirred at 313 K, under a nitrogen atmosphere for 1 h. To this mixture, a solution of 1,3,5-tris(bromomethyl)benzene (1.00 g, 2.80 mmol) in dry dimethylformamide (40 ml) was added dropwise, under a nitrogen atmosphere over a period of 2–3 h. The reaction mixture was stirred for 2 d at 313 K and then poured into ice–water (150 g). The product was filtered off and washed with (10% *w*/*m*) NaOH solution and water. Recrystallization from ethanol solution gave a white product (yield 0.38 g, 26%, m.p. 333 K). Single crystals were obtained from absolute ethanol at room temperature by slow evaporation. Elemental analysis calculated: C 82.72, H 8.10%; found: C 82.62, H 8.14%.

Crystal data

$C_{36}H_{42}O_3$
M_r = 522.70
Triclinic, $P\overline{1}$
a = 9.3172 (7) Å
b = 11.5055 (9) Å
c = 16.3424 (13) Å
α = 104.677 (6)°
β = 105.307 (6)°
γ = 103.098 (6)°
V = 1551.6 (2) Å^3
Z = 2
D_x = 1.119 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17053 reflections
θ = 1.4–27.1°
μ = 0.07 mm^{-1}
T = 298 (2) K
Prism, colorless
0.71 × 0.34 × 0.14 mm

Data collection

Stoe IPDS-II diffractometer
φ and ω scans
Absorption correction: by integration (*X-RED32*; Stoe amp; Cie, 2002)
T_{min} = 0.970, T_{max} = 0.992
21653 measured reflections
6830 independent reflections
2985 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.2°
$h = -10 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 0.85
6830 reflections
461 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.010 (2)

Table 1
Selected geometric parameters (Å, °).

C7—O1	1.420 (2)	C10—O1	1.3783 (19)
C8—O2	1.416 (2)	C19—O2	1.372 (2)
C9—O3	1.424 (2)	C28—O3	1.367 (2)
C10—O1—C7	117.57 (14)	C28—O3—C9	119.07 (15)
C19—O2—C8	117.42 (14)		
C1—C7—O1—C10	177.07 (16)	C5—C9—O3—C28	−179.86 (15)
C3—C8—O2—C19	−172.44 (16)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2	0.929 (18)	2.379 (17)	2.756 (2)	104.1 (13)
C4—H4···O3	0.942 (18)	2.305 (17)	2.695 (2)	104.2 (12)

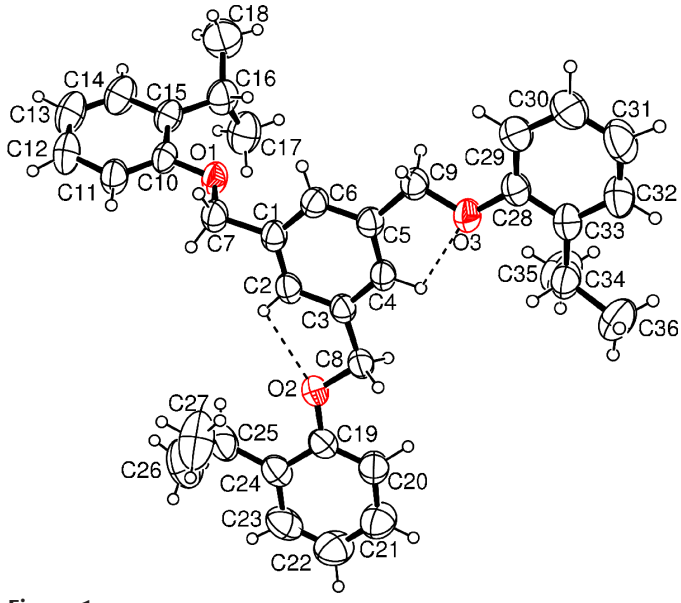


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and dashed lines indicate hydrogen bonds.

Methyl H atoms, except for those on atom C17, were positioned geometrically at a distance of 0.96 Å from the parent C atoms; a riding model was used during the refinement process and U_{iso}(H) values were constrained to be $1.5U_{eq}$(carrier atom). The other H atoms were located in a difference synthesis and refined freely [CH C—H = 0.93 (2)–1.04 (2) Å, CH_2 C—H = 0.97 (2)–1.03 (2) Å and U_{iso}(H) = 0.065 (5)–0.159 (11) Å^2].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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