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1-(4-Benzyloxyphenyl)-2-bromopropan-1-one

Song-Qing Wang,[a] Hong-Mei Zhao[a] and Xiu-Jie Liu[b]*

[a]School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Tianjin University of Technology, Tianjin 300191, People's Republic of China

Correspondence e-mail: hmzhao81@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.140
Data-to-parameter ratio = 19.2

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

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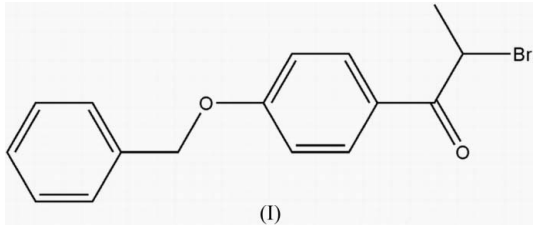
In the title compound, $C_{16}H_{15}BrO_2$, a key intermediate for the synthesis of possible selective estrogen receptor modulators, the dihedral angle between the benzene rings is 74.2 (2)°.

Comment

Bazedoxifene is a selective estrogen receptor modulator under investigation for the prevention and treatment of post-menopausal osteoporosis. It is also being studied in combination with estrogen replacement therapy for the treatment of the menopause and its associated symptoms. The title compound, (I) (Fig. 1), is an intermediate in the synthesis of bazedoxifene, and its structure is reported here. The dihedral angle between the two benzene-ring best planes (C4–C9 and C11–C16) is 74.2 (2)°.



(I)

A weak C—H···O interaction (Table 1) connects adjacent molecules into a zigzag chain along the [010] direction (Fig. 2). Within this one-dimensional motif, a short O2···Br1 interaction of 3.399 (3) Å also occurs.

Experimental

The title compound was prepared following a procedure described by Bockmuhl & Stein (1932). Colourless prismatic single crystals of (I) were obtained by recrystallization from chloroform (m.p. 353 K). Analysis calculated for $C_{16}H_{15}BrO_2$: C 60.21, H 4.74%; found: C 60.36, H 4.36%.

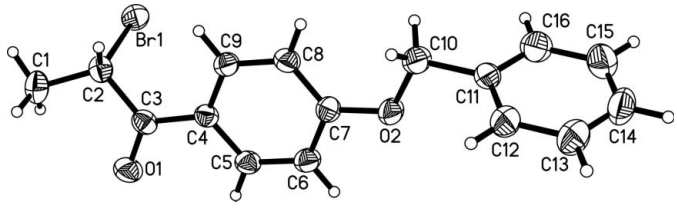


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

Crystal data

$C_{16}H_{15}BrO_2$
M_r = 319.19
Monoclinic, $P2_1/n$
a = 4.9306 (10) Å
b = 9.7622 (14) Å
c = 29.912 (6) Å
β = 90.861 (8)°
V = 1439.6 (5) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.85 mm^{-1}
T = 293 (2) K
Prism, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.548, T_{max} = 0.628
11828 measured reflections
3359 independent reflections
2354 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.140
S = 1.09
3359 reflections
175 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0138 (18)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.93	2.53	3.417 (5)	160

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

H atoms attached to C were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride during subsequent refinement with an isotropic displacement parameter fixed at 1.2 times U_{eq}(C) or 1.5 times U_{eq}(methyl C) of the parent atom.

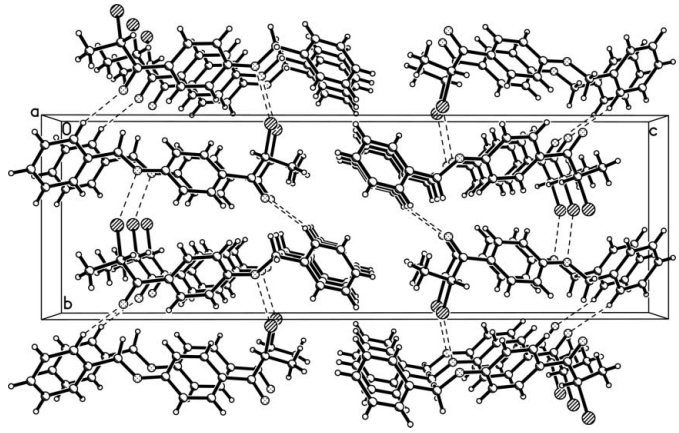


Figure 2
Packing diagram for (I), with C—H···O interactions and short O···Br contacts shown as dashed lines.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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