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2-Bromo-1-mesitylethanone

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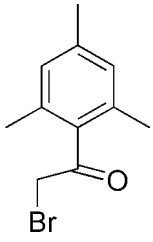
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.009 Å; R factor = 0.064; wR factor = 0.095; data-to-parameter ratio = 17.0.

In the molecule of the title compound, $C_{11}H_{13}BrO$, the adjacent C atoms are almost coplanar with the aromatic ring [maximum deviation 0.035 (3) Å]. In the crystal structure, weak intermolecular C—H···O interactions link the molecules into chains along the b axis. A very weak C—H···π interaction is also present.

Related literature

The title compound is used to synthesize organic electronic devices, see: Rose *et al.* (2008). For a related structure, see: Guss (1953). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{13}BrO$
M_r = 241.12
Orthorhombic, *Pbca*
a = 15.379 (3) Å
b = 8.2820 (17) Å
c = 17.374 (4) Å
V = 2212.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.68 mm^{-1}
T = 294 K
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.527, T_{max} = 0.710
3509 measured reflections
2002 independent reflections
805 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.095
S = 1.00
2002 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9B···O^{i}	0.96	2.52	3.462 (7)	166
C11—H11A···O^{i}	0.97	2.36	3.308 (7)	167
C7—H7C···$Cg1^{ii}$	0.96	2.94	3.722 (3)	140

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x, -y+1, -z+1$. $Cg1$ is the centroid of the C1–C6 ring.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2660).

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supporting information

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S1. Comment

The title compound is used to synthesize organic electronic devices and medical intermediates (Rose *et al.*, 2008). We report herein the crystal structure of the title compound, which is interested to us in the field.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C1-C6) is, of course, planar. Atoms C7, C8, C9 and C10 are -0.012 (2), -0.019 (3), -0.035 (3) and -0.006 (3) Å away from the ring plane of A, respectively.

In the crystal structure, weak intermolecular C-H···O interactions (Table 1) link the molecules into chains along the b axis, in which they may be effective in the stabilization of the structure. There also exists a weak C—H···π interaction (Table 1).

S2. Experimental

The title compound, (m.p. 323-324 K), was prepared according to the literature method (Guss, 1953). Crystals suitable for X-ray analysis were obtained by dissolving the title compound (0.2 g) in ethyl acetate (50 ml) and evaporating the solvent slowly at room temperature for about 3 d.

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

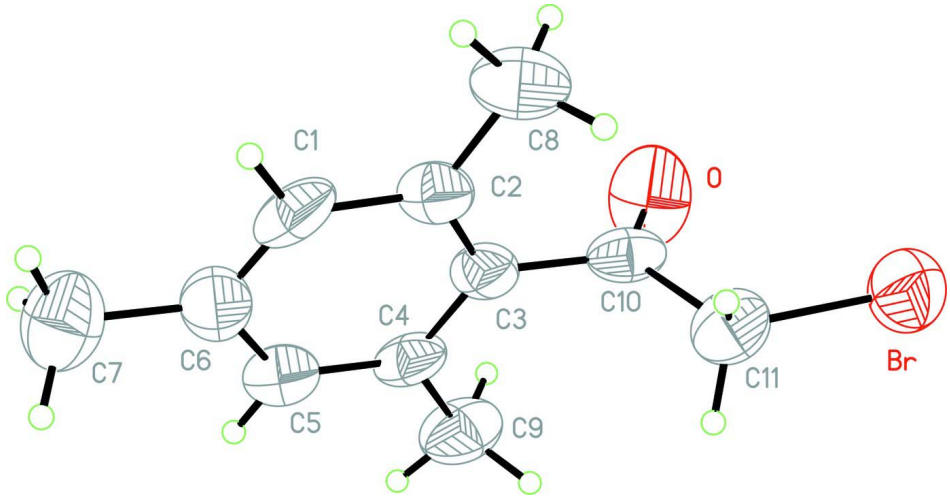

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

2-bromo-1-mesitylethanone

Crystal data

$C_{11}H_{13}BrO$
$M_r = 241.12$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 15.379\ (3)$ Å
$b = 8.2820\ (17)$ Å
$c = 17.374\ (4)$ Å
$V = 2212.9\ (8)$ Å^3
$Z = 8$
$F(000) = 976$
$D_x = 1.447$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–$13°$
$\mu = 3.68$ mm^{-1}
$T = 294$ K
Needle, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.527$, $T_{max} = 0.710$
3509 measured reflections
2002 independent reflections
805 reflections with $I > 2\sigma(I)$
$R_{int} = 0.099$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.3°$
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 9$
$l = -20 \rightarrow 12$
3 standard reflections every 120 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.095$
$S = 1.00$
2002 reflections
118 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br	0.22106 (4)	0.01688 (8)	0.59900 (4)	0.0758 (3)
O	0.1783 (3)	−0.1396 (5)	0.7510 (3)	0.0853 (16)
C1	−0.0250 (4)	0.1475 (7)	0.8818 (4)	0.0557 (19)
H1A	−0.0852	0.1583	0.8816	0.067*
C2	0.0138 (4)	0.0860 (6)	0.8160 (4)	0.0461 (16)
C3	0.1038 (4)	0.0675 (6)	0.8208 (4)	0.0458 (17)
C4	0.1509 (4)	0.1135 (7)	0.8840 (4)	0.0462 (17)
C5	0.1083 (4)	0.1744 (7)	0.9464 (4)	0.0540 (18)
H5A	0.1400	0.2040	0.9898	0.065*
C6	0.0180 (5)	0.1932 (7)	0.9465 (4)	0.062 (2)
C7	−0.0290 (3)	0.2598 (7)	1.0151 (4)	0.079 (2)
H7A	−0.0903	0.2624	1.0048	0.119*
H7B	−0.0088	0.3672	1.0255	0.119*
H7C	−0.0181	0.1924	1.0590	0.119*
C8	−0.0388 (3)	0.0364 (6)	0.7488 (3)	0.0630 (18)
H8A	−0.0989	0.0601	0.7583	0.094*
H8B	−0.0319	−0.0774	0.7403	0.094*
H8C	−0.0196	0.0944	0.7040	0.094*
C9	0.2492 (3)	0.0917 (7)	0.8895 (3)	0.068 (2)
H9A	0.2692	0.1304	0.9385	0.101*
H9B	0.2769	0.1517	0.8491	0.101*
H9C	0.2633	−0.0207	0.8843	0.101*
C10	0.1514 (4)	−0.0002 (8)	0.7513 (3)	0.0459 (15)
C11	0.1681 (3)	0.1137 (7)	0.6882 (3)	0.0592 (19)
H11A	0.2057	0.1991	0.7069	0.071*
H11B	0.1135	0.1628	0.6729	0.071*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0835 (6)	0.0705 (5)	0.0734 (5)	−0.0009 (5)	0.0146 (4)	−0.0066 (5)
O	0.111 (4)	0.057 (3)	0.088 (4)	0.040 (3)	0.016 (3)	0.015 (3)

C1	0.033 (4)	0.044 (4)	0.090 (6)	0.000 (3)	0.021 (4)	0.011 (4)
C2	0.037 (5)	0.036 (4)	0.065 (5)	0.002 (3)	0.000 (4)	−0.005 (4)
C3	0.044 (5)	0.030 (4)	0.064 (5)	−0.002 (3)	0.011 (4)	−0.009 (3)
C4	0.026 (4)	0.041 (4)	0.072 (6)	−0.004 (3)	0.005 (4)	0.001 (4)
C5	0.047 (5)	0.050 (4)	0.065 (5)	−0.008 (4)	−0.004 (4)	0.002 (4)
C6	0.087 (7)	0.039 (4)	0.059 (6)	−0.005 (5)	0.016 (5)	0.002 (4)
C7	0.075 (6)	0.084 (5)	0.079 (7)	0.015 (4)	0.011 (5)	0.009 (5)
C8	0.049 (4)	0.054 (4)	0.085 (5)	0.000 (4)	−0.021 (4)	0.002 (4)
C9	0.048 (5)	0.080 (5)	0.075 (5)	−0.016 (3)	−0.015 (4)	0.014 (4)
C10	0.038 (4)	0.038 (4)	0.061 (4)	−0.005 (4)	−0.016 (3)	0.010 (5)
C11	0.042 (4)	0.065 (5)	0.070 (5)	0.002 (3)	0.003 (4)	0.003 (4)

Geometric parameters (Å, º)

Br—C11	1.925 (6)	C6—C7	1.499 (8)
O—C10	1.226 (6)	C7—H7A	0.9600
C1—C6	1.358 (9)	C7—H7B	0.9600
C1—C2	1.387 (8)	C7—H7C	0.9600
C1—H1A	0.9300	C8—H8A	0.9600
C2—C3	1.396 (7)	C8—H8B	0.9600
C2—C8	1.479 (7)	C8—H8C	0.9600
C3—C4	1.369 (8)	C9—H9A	0.9600
C3—C10	1.519 (8)	C9—H9B	0.9600
C4—C5	1.364 (7)	C9—H9C	0.9600
C4—C9	1.526 (7)	C10—C11	1.470 (7)
C5—C6	1.399 (7)	C11—H11A	0.9700
C5—H5A	0.9300	C11—H11B	0.9700
C6—C1—C2	125.2 (6)	H7B—C7—H7C	109.5
C6—C1—H1A	117.4	C2—C8—H8A	109.5
C2—C1—H1A	117.4	C2—C8—H8B	109.5
C1—C2—C3	114.7 (6)	H8A—C8—H8B	109.5
C1—C2—C8	121.2 (6)	C2—C8—H8C	109.5
C3—C2—C8	124.0 (6)	H8A—C8—H8C	109.5
C4—C3—C2	122.8 (6)	H8B—C8—H8C	109.5
C4—C3—C10	119.0 (6)	C4—C9—H9A	109.5
C2—C3—C10	118.1 (6)	C4—C9—H9B	109.5
C5—C4—C3	119.1 (6)	H9A—C9—H9B	109.5
C5—C4—C9	118.0 (6)	C4—C9—H9C	109.5
C3—C4—C9	122.8 (6)	H9A—C9—H9C	109.5
C4—C5—C6	121.3 (6)	H9B—C9—H9C	109.5
C4—C5—H5A	119.4	O—C10—C11	122.8 (6)
C6—C5—H5A	119.4	O—C10—C3	120.9 (5)
C1—C6—C5	116.8 (7)	C11—C10—C3	116.1 (6)
C1—C6—C7	121.8 (7)	C10—C11—Br	114.0 (4)
C5—C6—C7	121.4 (8)	C10—C11—H11A	108.7
C6—C7—H7A	109.5	Br—C11—H11A	108.7
C6—C7—H7B	109.5	C10—C11—H11B	108.7

H7A—C7—H7B	109.5	Br—C11—H11B	108.7
C6—C7—H7C	109.5	H11A—C11—H11B	107.6
H7A—C7—H7C	109.5		
C6—C1—C2—C3	2.1 (9)	C9—C4—C5—C6	−178.0 (5)
C6—C1—C2—C8	178.8 (6)	C2—C1—C6—C5	−0.8 (10)
C1—C2—C3—C4	−3.0 (8)	C2—C1—C6—C7	179.6 (6)
C8—C2—C3—C4	−179.6 (6)	C4—C5—C6—C1	0.2 (9)
C1—C2—C3—C10	179.6 (5)	C4—C5—C6—C7	179.9 (6)
C8—C2—C3—C10	3.0 (8)	C4—C3—C10—O	77.5 (8)
C2—C3—C4—C5	2.6 (9)	C2—C3—C10—O	−105.0 (7)
C10—C3—C4—C5	180.0 (5)	C4—C3—C10—C11	−98.3 (6)
C2—C3—C4—C9	179.4 (5)	C2—C3—C10—C11	79.2 (7)
C10—C3—C4—C9	−3.3 (8)	O—C10—C11—Br	8.5 (8)
C3—C4—C5—C6	−1.2 (9)	C3—C10—C11—Br	−175.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*B*···O^{i}	0.96	2.52	3.462 (7)	166
C11—H11*A*···O^{i}	0.97	2.36	3.308 (7)	167
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Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*; (ii) −*x*, −*y*+1, −*z*+1.