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5-Methoxyindan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.124
Data-to-parameter ratio = 13.5

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

The title compound, $C_{10}H_{10}O_2$, is an important intermediate for the preparation of biologically active compounds. The molecule is planar and weak C—H···O hydrogen bonding helps to stabilize the crystal structure.

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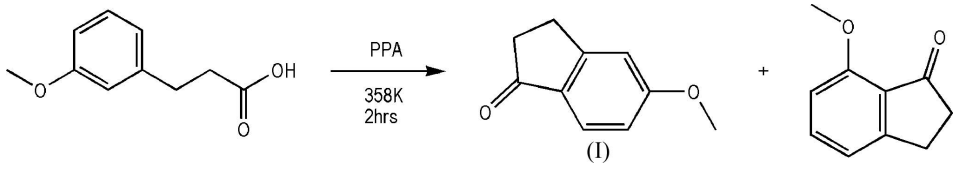
Comment

1-Indanones are important synthetic intermediates for pharmaceuticals and biologically active compounds (Bogeso *et al.*, 1995; Guillon *et al.*, 2002) and ligands of olefin polymerization catalysts (Schumann *et al.*, 2001; Herzog *et al.*, 2002). The synthesis of the title compound, (I), and crystallographic cell dimensions of its crystal were reported by Cooper *et al.* (2003). We present here the crystal structure of (I).



(I)

The molecule of (I) is planar (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Weak C—H···O hydrogen bonding helps to stabilize the crystal structure of (I) (Table 1).

Experimental

3-(3-Methoxyphenyl)propionic acid (15 g) was dissolved in hot polyphosphoric acid (250 g, 358 K). The resulting yellow solution was heated on an oil bath with stirring for 2 h. The cooled solution was added to 500 ml of ice–water. The mixture was extracted with three 150 ml portions of ethyl acetate and the combined extracts washed with 5% sodium hydroxide solution and then with water until the washings were neutral. The ethyl acetate solution was dried over

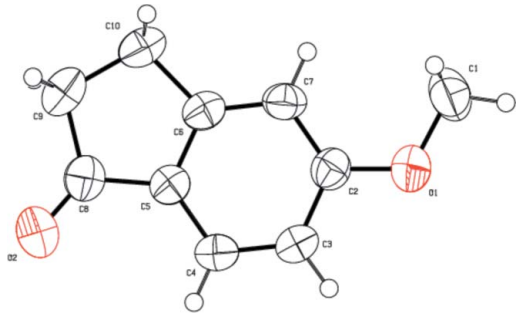


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

magnesium sulfate. The organic layer was concentrated and chromatographed on silica gel using petroleum ether (313–353 K) as eluant to afford (I) (8.8 g, 77%). Colorless single crystals of (I) were obtained by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{10}H_{10}O_2$
M_r = 162.18
Monoclinic, $P2_1/c$
a = 7.4114 (7) Å
b = 10.6122 (10) Å
c = 10.9137 (10) Å
β = 103.692 (2)°
V = 833.98 (13) Å^3
Z = 4
D_x = 1.292 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colorless
0.40 × 0.28 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
ω and φ scans
Absorption correction: none
4004 measured reflections
1468 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.124
S = 1.01
1468 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 0.0604P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O2^{i}	0.96	2.41	3.366 (2)	171
C3—H3A···O2^{ii}	0.93	2.52	3.4162 (17)	161

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

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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