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1-(2-Furyl)-3-hydroxy-3-(2-methoxy-2-naphthyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.056
wR factor = 0.138
Data-to-parameter ratio = 15.1

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

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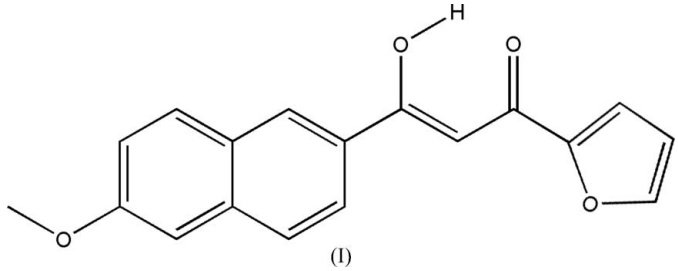
Molecules of the title compound, $C_{18}H_{14}O_4$, crystallize as the enol tautomer, containing an intramolecular O—H···O hydrogen bond. The entire molecule is approximately planar.

Comment

1,3-Diketones possess a broad spectrum of useful and sometimes unique chemical properties, which make them extremely attractive as synthetic intermediates. They are also used widely for the preparation of metallocomplexes (Gorczynski *et al.*, 2005; Liang *et al.*, 2003). Molecular crystals of 1,3-diketones are found to comprise enol tautomers, stabilized by a strong intramolecular O—H···O hydrogen bond (Bertolasi *et al.*, 1991; Gilli *et al.*, 2004; Vila *et al.*, 1991).



(I)

The title compound, (I) (Fig. 1), crystallizes as the enol tautomer, forming the expected intramolecular O—H···O hydrogen bond (Table 1). The entire molecule is approximately planar. The dihedral angles between the two aromatic rings (C16/C17/C18/O4/C15 and C5/C6/C11/C10/C9/C8) is 5.42 (5)°. The two adjacent six-membered rings in the naphthyl system are almost coplanar and the dihedral angles between them is 1.02 (4)°.

Experimental

1-(2-Methoxynaphthalen-6-yl)ethanone (6.00 g, 0.03 mol), methyl-furan-2-carboxylate (3.78 g, 0.03 mol), $NaNH_2$ (1.37 g, 0.035 mol) and dry diethyl ether (40 ml) were stirred for 6 h at room temperature under a nitrogen atomosphere. The reaction mixture was then acidified with dilute hydrochloric acid (*ca* 10 ml), and the ether layer was separated, washed with saturated $NaHCO_3$ solution (40 ml) and dried over anhydrous Na_2SO_4. The solvent was removed by evaporation and the residual solid was recrystallized from ethanol (100 ml) to give the title compound (yield 4.86 g, 55.1%, m.p. 414 K). Crystals suitable for X-ray diffraction were grown by slow evaporation of a CH_2Cl_2/EtOH (2:1) solution at room temperature.

Crystal data

$C_{18}H_{14}O_4$
M_r = 294.29
Monoclinic, $P2_1/c$
a = 3.9333 (7) Å
b = 10.986 (2) Å
c = 33.046 (6) Å
β = 90.956 (3)°
V = 1427.8 (4) Å^3
Z = 4
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Plate, yellow
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.972, T_{max} = 0.989
8120 measured reflections
3064 independent reflections
2599 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.138
S = 1.07
3064 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.3755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3	0.98 (2)	1.55 (2)	2.4899 (18)	158 (2)

H atoms bound to C atoms were included in idealized positions, with C—H = 0.93 (aromatic) or 0.96 Å (methyl), and allowed to ride during subsequent refinement, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl group was also allowed to rotate about its local threefold axis. Atom H2 of the hydroxyl group was located in a difference Fourier map and its position was refined freely, with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

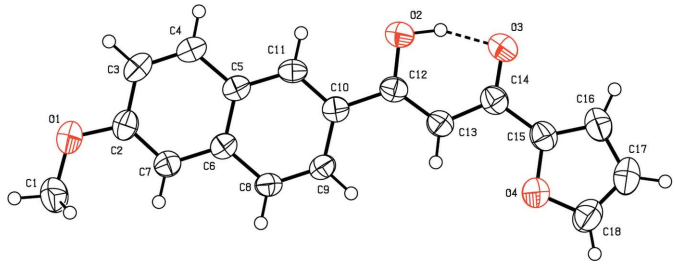


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms. The dashed line indicates the intramolecular O—H···O hydrogen bond.

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