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(±)-(3a*R*,4*R*,4a*S*)-4-Phenyl-3,3a,4,4a-tetrahydro-1*H*-cyclopropa[*c*]furan-1-one

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Key indicators

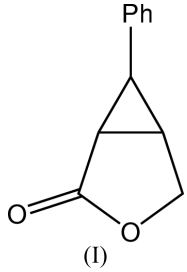
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.144
Data-to-parameter ratio = 16.6

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

The furanone ring in the title compound, $C_{11}H_{10}O_2$, is effectively planar and forms a dihedral angle of 74.42 (14)° with the cyclopropyl ring. The phenyl ring is somewhat twisted with respect to the approximate 'mirror plane' of the bicyclic system; the dihedral angles formed by the plane of the phenyl ring with the cyclopropyl and furanone mean planes are almost equal, *viz*. 98.30 (14) and 98.14 (10)°, respectively.

Comment

The title compound, (I), was prepared by the cyclization of 2-(hydroxymethyl)-3-phenylcyclopropane-1-carboxylic acid (Avery *et al.*, 2001). An enantiomerically pure form of the compound has been reported previously (Doyle *et al.*, 1995); the structure of the racemic crystal was determined in the present work (a view of the molecule with the atomic numbering is given in Fig. 1).



(I)

The deviations of the O2, C1, C3, C3a and C4a atoms from their least-squares plane are 0.080 (1), −0.056 (2), −0.068 (2), 0.035 (2) and 0.009 (2) Å, respectively; for reference, the displacement of the C4 atom from this plane is 1.285 (2) Å. The dihedral angle formed by the five-membered ring and the plane through the cyclopropyl ring is 74.42 (14)°. The phenyl ring is somewhat twisted with respect to the approximate 'mirror plane' of the bicyclic system; the dihedral angles formed by the plane of the phenyl ring with the cyclopropyl and furanone mean planes are, quite expectedly, almost equal [98.30 (14) and 98.14 (10)°, respectively], and the C4a—C4—C41—C42 torsion angle is 152.59 (17)°. The twist about the C4—C41 bond presumably allows for the minimization of the total energy associated with short intramolecular H···H contacts involving H atoms at the C4, C3a, C4a, C42 and C46 atoms.

Experimental

The title compound was prepared by the trifluoroacetic acid-catalysed cyclization of the 2-(hydroxymethyl)-3-phenylcyclopropane-1-carboxylic acid precursor as described previously (Avery *et al.*, 2001).

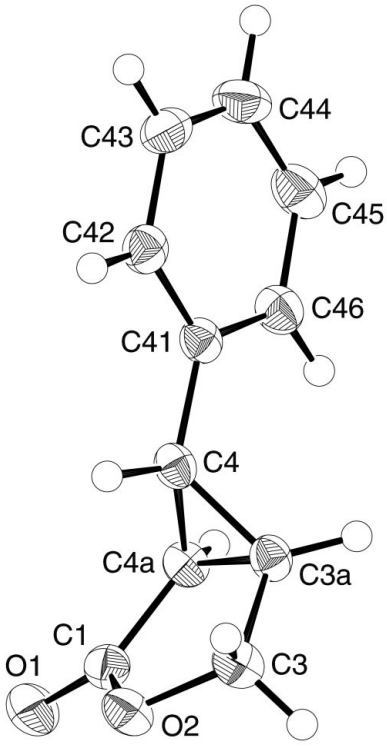


Figure 1
The molecular structure and crystallographic numbering scheme for (I). Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

Crystals were obtained from the slow evaporation of a heptane solution of the compound; m.p. 367–369 K.

Crystal data

$C_{11}H_{10}O_2$
$M_r = 174.20$
Monoclinic, $P2_1/n$
$a = 8.927\ (1)$ Å
$b = 10.2311\ (9)$ Å
$c = 9.776\ (2)$ Å
$\beta = 106.04\ (2)^\circ$
$V = 858.1\ (2)$ Å^3
$Z = 4$
$D_x = 1.348$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 7.4$–12.9°
$\mu = 0.09$ mm^{-1}
$T = 173$ K
Plate, pale yellow
$0.45 \times 0.39 \times 0.07$ mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
2215 measured reflections
1975 independent reflections
1205 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5^\circ$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 13$
$l = -12 \rightarrow 12$
3 standard reflections
every 400 reflections
intensity decay: 0.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.144$
$S = 0.93$
1975 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

H atoms were placed in geometrically calculated positions and included in the final refinement in the riding model approximation with an overall displacement parameter.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1996); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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