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#### Key indicators

Single-crystal X-ray study

$T = 150$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å

$R$  factor = 0.039

$wR$  factor = 0.095

Data-to-parameter ratio = 13.7

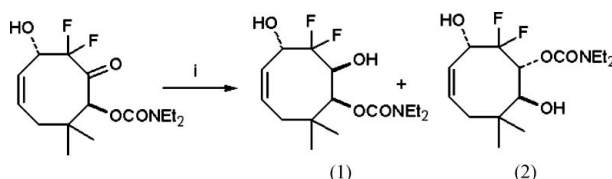
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## (1*R*\*,3*S*\*,8*S*\*)-2,2-Difluoro-3,8-dihydroxy-5,5-dimethylcyclooct-4(*Z*)-en-1-yl *N,N*-diethylcarbamate

The structure of the title compound,  $\text{C}_{15}\text{H}_{25}\text{F}_2\text{NO}_4$ , is presented. Comparison of this minor product with the isomeric major product of the synthesis is made in the previous paper.

### Comment

The pseudorotational relationship between the ring conformations of the title compound, (2), and diol (1), which was presented in the previous paper (Fawcett *et al.*, 2005), are discussed in the *Comment* of that paper.



Hydrogen bonding (Table 1) links molecules of (2) into sheets perpendicular to the *c* axis.

### Experimental

Compound (2) was obtained as the minor product during the preparation of diol (1), as described in the previous paper (Fawcett *et al.*, 2005). A sample was recrystallized by vapour diffusion (ethyl acetate/light petroleum) to afford colourless crystals.

#### Crystal data

$\text{C}_{15}\text{H}_{25}\text{F}_2\text{NO}_4$

$M_r = 321.36$

Monoclinic,  $P2_1/c$

$a = 20.062$  (14) Å

$b = 6.433$  (4) Å

$c = 12.424$  (9) Å

$\beta = 97.346$  (12)°

$V = 1590.4$  (19) Å<sup>3</sup>

$Z = 4$

$D_x = 1.342$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

Cell parameters from 3558 reflections

$\theta = 3.1$ – $28.1$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 150$  (2) K

Block, colourless

$0.28 \times 0.22 \times 0.15$  mm

#### Data collection

Bruker APEX CCD area-detector diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: none

10968 measured reflections

2805 independent reflections

2413 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.068$

$\theta_{\text{max}} = 25.0$ °

$h = -23 \rightarrow 23$

$k = -7 \rightarrow 7$

$l = -14 \rightarrow 14$

#### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.095$

$S = 1.05$

2805 reflections

205 parameters

H-atom parameters constrained

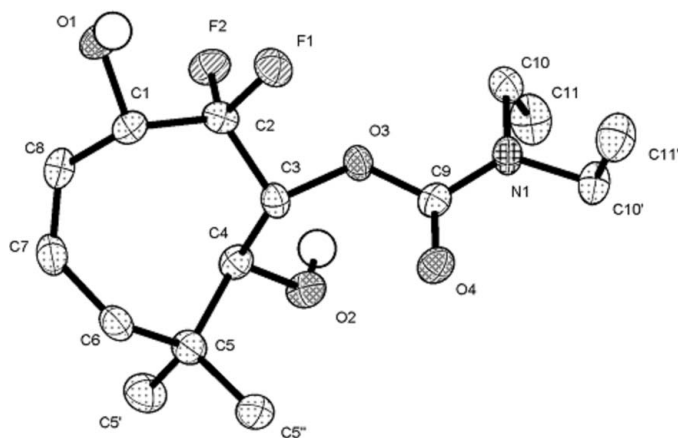
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.1172P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.003$

$\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>



**Figure 1**  
The molecular structure of (2), showing the atom-numbering scheme and 50% displacement ellipsoids. H atoms have been omitted.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1\cdots O4^i$	0.84	1.92	2.7598 (19)	173
$O2-H2\cdots O1^{ii}$	0.84	2.01	2.827 (2)	163

Symmetry codes: (i)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (ii)  $x, -y + \frac{1}{2}, z - \frac{1}{2}$ .

H atoms were positioned geometrically, with  $C-H = 0.95-1.00 \text{ \AA}$  and  $O-H = 0.84 \text{ \AA}$ , and treated as riding, with  $U_{iso}(H) = 1.2$  or  $1.5$  (methyl and OH) times  $U_{eq}$  of the parent atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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