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1,2-Di-2-thienyl-2-hydroxyethanone (2,2′-thenoin)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.048
wR factor = 0.172
Data-to-parameter ratio = 9.3

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

The title compound, $C_{10}H_8O_2S_2$, is the 2-thienyl symmetric analog of benzoin. 2,2′–Thenoin can be synthesized in good yield utilizing the benzoin condensation reaction (starting with 2-thiophenecarboxaldehyde). The crystal structure of 2,2′-thenoin has been determined at room temperature.

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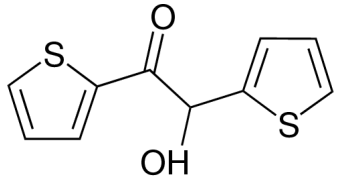
Comment

2,2′-Thenoin, (I) (Fig. 1), crystallizes with one molecule in the asymmetric unit and forms cyclical hydrogen-bonded dimers. The hydrogen-bond distance is 2.07 Å [for O2—H2*A*···O1^{i} and O1···H2*A*^{i}–O2^{i}; symmetry code (i) 1−*x*, 1/2+*y*, 1/2−*z*].



(I)

Experimental

2,2′-Thenoin is a symmetrically substituted thienyl analog of benzoin (Cardon & Lankelma, 1948). It can be prepared in adequate yield using the benzoin condensation reaction commonly encountered in undergraduate organic laboratory texts (Pavia *et al.*, 1998). Recrystallization from boiling 95% ethanol yielded colorless plates of 2,2′-thenoin (m.p. 390–391 K). IR (Fluoromac, cm^{-1}): 3400 (*s* and *b*), 3100 (*m*), 2950 (*m*), 2850 (*m*); IR (Nujol, cm^{-1}): 1700 (*s*), 1450 (*m*), 1380 (*s*), 1070 (*s*); ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.71 (*m*, 2H), 7.09 (*m*, 2H), 6.95 (*m*, 2H), 6.01 (*s*, 1H), 4.20 (*s*, 1H). The melting point determined in this study is 10 K higher than for the compound initially reported in the literature (Cardon & Lankelma, 1948). However, other molecules with melting points mentioned in that paper were synthesized in our laboratory and our values agree with theirs.

Compound (I)

Crystal data

$C_{10}H_8O_2S_2$
M_r = 224.28
Monoclinic, $P2_1/c$
a = 10.8436 (11) Å
b = 6.0348 (6) Å
c = 16.336 (2) Å
β = 110.001 (2)°
V = 1004.55 (19) Å^3
Z = 4
D_x = 1.483 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3834 reflections
θ = 2.0–23.3°
μ = 0.50 mm^{-1}
T = 294 (2) K
Rhomb, colorless
0.2 × 0.1 × 0.1 mm

Data collection

Siemens SMART P3/512-CCD diffractometer	$R_{int} = 0.038$
	$\theta_{max} = 21.7^\circ$
ω scans	$h = -11 \rightarrow 5$
3645 measured reflections	$k = -6 \rightarrow 6$
1183 independent reflections	$l = -14 \rightarrow 17$
1010 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.173$	
$S = 1.37$	$(\Delta/\sigma)_{max} = 0.003$
1183 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
127 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

S1—C5	1.668 (5)	C2—C3	1.390 (6)
S1—C2	1.721 (4)	C3—C4	1.409 (6)
O1—C1	1.214 (5)	C4—C5	1.357 (7)
C1—C2	1.468 (6)	C6—C7	1.495 (6)
C1—C6	1.533 (6)	C7—C8	1.403 (6)
S2—C10	1.691 (6)	C8—C9	1.410 (7)
S2—C7	1.710 (4)	C9—C10	1.324 (7)
O2—C6	1.419 (5)		
C5—S1—C2	91.6 (2)	C4—C5—S1	113.6 (3)
O1—C1—C2	121.4 (4)	O2—C6—C7	112.6 (3)
O1—C1—C6	121.3 (4)	O2—C6—C1	106.9 (3)
C2—C1—C6	117.3 (4)	C7—C6—C1	110.3 (3)
C10—S2—C7	92.3 (3)	C8—C7—C6	128.3 (4)
C3—C2—C1	130.1 (4)	C8—C7—S2	110.2 (3)
C3—C2—S1	111.3 (3)	C6—C7—S2	121.5 (3)
C1—C2—S1	118.7 (3)	C7—C8—C9	110.9 (4)
C2—C3—C4	111.0 (4)	C10—C9—C8	114.0 (5)
C5—C4—C3	112.6 (4)	C9—C10—S2	112.5 (4)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

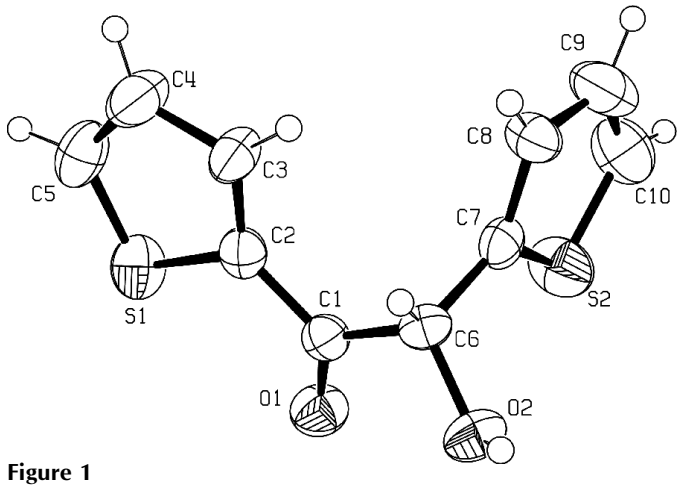


Figure 1
The molecular structure of 2,2′-thenoin, showing 50% probability displacement ellipsoids.

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