The structure of the title compound, \( \text{C}_8\text{H}_{10}\text{O}_3\text{S} \), (I), has been determined as part of an investigation into the synthesis and characterization of \( \alpha \)-hydroxy sulfones. Compound (I) is novel and its X-ray structure is the first recorded for a simple \( \alpha \)-hydroxy sulfone. In the crystals of (I), pairs of molecules are linked by intermolecular O–H···O sulfonyl hydrogen bonds around a centre of symmetry to form a dimer.

Comment

The title compound, (I), is an \( \alpha \)-hydroxy sulfone. It was obtained as a crystalline compound which decomposed very slowly upon standing. This result was considered unusual in that simple \( \alpha \)-hydroxy sulfones such as this have been reported as being unstable and easily subject to cleavage (Field & Settlage, 1951; Bredereck et al., 1954). In the crystals, pairs of centrosymmetrically related molecules are associated through intermolecular hydrogen-bonding interactions between the \( \alpha \)-hydroxyl groups and one of the sulfone O atoms so as to form a dimer \([\text{H} \cdots \text{O}^3 \doteq 1.99 \text{ Å}, \text{O}^1 \cdots \text{O}^3 \doteq 2.783 (4) \text{ Å} \text{ and } \text{O}^1 \cdots \text{H} \cdots \text{O}^3 \doteq 161^\circ; \text{symmetry code: } (i) -x, 1-y, 1-z]\). This hydrogen-bonding motif can be described using graph-set notation (Bernstein et al., 1995) as \( R_{2}^{2}(10) \). The S1–C1 bond distance of 1.799 (3) Å is 0.02 Å longer than the S1–C2 bond distance of 1.779 (3) Å. This is consistent with the influence of the electron-withdrawing O atom attached to atom C1.

Experimental

The title compound was prepared by the reaction of benzylmagnesium chloride with sulfur dioxide followed by quenching with sulfuric acid to yield benzylsulfinic acid (van Allen et al., 1966). Immediate treatment with formaldehyde (Bredereck & Bäder, 1954) yielded (I) upon work-up as a solid powder. Crystals were isolated as colourless needles by slow evaporation of an ether solution of (I).
Crystal data
C₈H₁₀O₃S
Mr = 186.23
Monoclinic, P2₁/n
a = 22.758 (11) Å
b = 7.160 (7) Å
(2) Å
β = 91.88 (3)
V = 883.0 (10) Å³
Z = 4
Dx = 1.401 Mg m⁻³
Mo Kα radiation
Cell parameters from 25 reflections
θ = 12.6–17.4°
μ = 0.33 mm⁻¹
T = 295 K
Prismatic, colourless
0.30 x 0.20 x 0.15 mm

Data collection
Rigaku AFC-7R diffractometer
ω/2θ scans
1795 measured reflections
1565 independent reflections
1155 reflections with I > 2σ(I)
Rint = 0.022
θmax = 25.0°

Refinement
Refinement on F²
R(F² > 2σ(F²)) = 0.036
wR(F²) = 0.101
S = 1.05
1565 reflections
109 parameters
H-atom parameters constrained

H atoms were placed at calculated positions with C—H distances set to 0.95 Å, except for the hydroxyl H atom, which was located from a difference synthesis, and O—H was set to 0.82 Å. All H atoms were constrained in the refinement.

Data collection: MSC/AFC-7 Diffractometer Control Software (Molecular Structure Corporation, 1999); cell refinement: MSC/AFC-7 Diffractometer Control Software; data reduction: teXsan for Windows (Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: teXsan for Windows; program(s) used to refine structure: teXsan for Windows and SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2001) and ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: teXsan for Windows and PLATON.

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References