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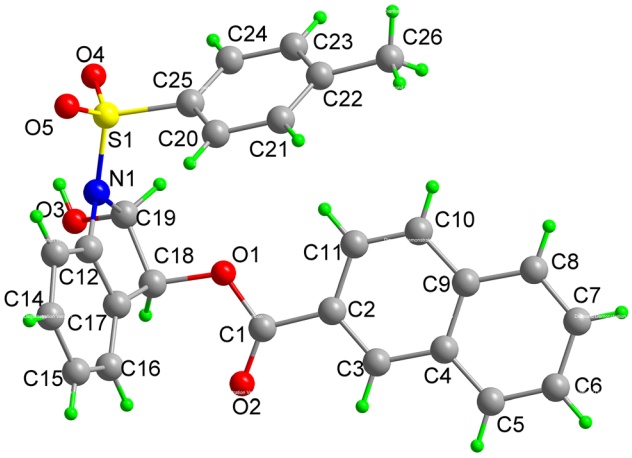
Crystal structure of 2-hydroxy-1-tosylindolin-3-yl-2-naphthoate, $C_{26}H_{21}N_1S_1O_5$



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Abstract

$C_{26}H_{21}N_1S_1O_5$, monoclinic, $P2_1/c$ (no. 14), a = 7.623(3) Å, b = 25.617(12) Å, c = 11.775(5) Å, β = 100.073(8)°, V = 2264.2(17) Å^3, Z = 4, $R_{gt}(F)$ = 0.0470, $wR_{ref}(F^2)$ = 0.1365, T = 298(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.23 × 0.20 × 0.12 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.18 mm^{-1}
Diffractometer, scan mode:	Bruker APEX, φ and ω
θ_{max}, completeness:	26.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,292, 4587, 0.032
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3363
$N(param)_{refined}$:	298
Programs:	SHELX [1], OLEX2 [2], CRYSALIS^{PRO} [3]

Source of material

The title compound was be synthesized using *trans*-2-hydroxy-1-tosylindoline-3-ammonium bromide [4–6] and commercial available 2-naphthoic acid stirred at 373 K for 8 h in ethyl acetate solution. The solution was cooled to room temperature, which was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1) to afford the product as a white solid. The crude product was recrystallized from ethyl acetate.

Experimental details

All H atoms were positioned geometrically and treated as riding, with C–H bond lengths constrained to 0.96° for methyl H atoms, 0.93° for phenyl H atoms, 0.82° for hydroxyl H atoms, with U_{iso}(H) = 1.2 U_{eq}(C) for CH groups, and hydroxyl atoms, and phenyl H atoms, and 1.5U_{eq}(C) for methyl H atoms.

Comment

Indoles are structural scaffolds frequently found in important pharmaceuticals and biologically active natural compounds. For example, 1*H*-indol-3-yl acetates are important materials for the preparation of biochemical reagents for the identification of campylobacte [7]. There is one molecule in the asymmetric unit of the title structure (see the figure). Bond lengths and angles are all

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1	0.20654 (6)	0.42815 (2)	0.62890 (4)	0.05140 (17)
N1	0.08166 (19)	0.44465 (5)	0.72203 (12)	0.0479 (4)
O1	−0.19596 (16)	0.36414 (4)	0.77700 (10)	0.0492 (3)
O2	−0.3400 (2)	0.35664 (5)	0.92738 (12)	0.0662 (4)
O3	−0.18949 (17)	0.49181 (5)	0.66884 (10)	0.0601 (4)
H3A	−0.159611	0.503996	0.610708	0.090*
O4	0.1227 (2)	0.45117 (5)	0.52270 (12)	0.0734 (5)
O5	0.38630 (18)	0.44113 (6)	0.67757 (15)	0.0741 (4)
C1	−0.2778 (2)	0.33663 (7)	0.85025 (14)	0.0473 (4)
C2	−0.2815 (2)	0.27996 (7)	0.82437 (14)	0.0448 (4)
C3	−0.3489 (2)	0.24645 (7)	0.89787 (14)	0.0464 (4)
H3B	−0.389240	0.259928	0.961968	0.056*
C4	−0.3577 (2)	0.19178 (7)	0.87752 (14)	0.0455 (4)
C5	−0.4237 (3)	0.15641 (7)	0.95265 (16)	0.0565 (5)
H5B	−0.462332	0.169033	1.018095	0.068*
C6	−0.4312 (3)	0.10409 (8)	0.93024 (19)	0.0675 (6)
H6A	−0.474571	0.081447	0.980520	0.081*
C7	−0.3742 (3)	0.08438 (9)	0.8324 (2)	0.0750 (6)
H7A	−0.380589	0.048709	0.817562	0.090*
C8	−0.3091 (3)	0.11710 (8)	0.75829 (19)	0.0715 (6)
H8A	−0.271584	0.103459	0.693347	0.086*
C9	−0.2977 (3)	0.17186 (7)	0.77908 (15)	0.0525 (5)
C10	−0.2290 (3)	0.20742 (8)	0.70580 (16)	0.0614 (5)
H10A	−0.188766	0.194703	0.640962	0.074*
C11	−0.2201 (3)	0.25927 (7)	0.72729 (15)	0.0534 (5)
H11A	−0.173156	0.281482	0.677762	0.064*
C12	0.1302 (3)	0.44137 (7)	0.84494 (15)	0.0485 (4)
C13	0.2956 (3)	0.45032 (8)	0.9137 (2)	0.0710 (6)
H13A	0.396201	0.457214	0.881538	0.085*
C14	0.3039 (4)	0.44852 (9)	1.0319 (2)	0.0869 (8)
H14A	0.413218	0.453302	1.079937	0.104*
C15	0.1554 (4)	0.43988 (8)	1.08009 (19)	0.0795 (8)
H15A	0.164693	0.440005	1.159897	0.095*
C16	−0.0081 (3)	0.43097 (7)	1.01112 (16)	0.0637 (6)
H16A	−0.108688	0.425154	1.044049	0.076*
C17	−0.0203 (3)	0.43081 (6)	0.89223 (14)	0.0477 (4)
C18	−0.1754 (2)	0.42023 (6)	0.79728 (14)	0.0460 (4)
H18A	−0.285486	0.436547	0.812048	0.055*
C19	−0.1162 (2)	0.44213 (7)	0.68971 (14)	0.0449 (4)
H19A	−0.152283	0.419129	0.623230	0.054*
C20	0.2708 (3)	0.32747 (7)	0.69876 (17)	0.0585 (5)
H20A	0.321150	0.341193	0.770168	0.070*
C21	0.2714 (3)	0.27410 (8)	0.6793 (2)	0.0700 (6)
H21A	0.321934	0.252058	0.738908	0.084*
C22	0.1990 (3)	0.25287 (8)	0.5740 (2)	0.0722 (6)
C23	0.1206 (3)	0.28589 (9)	0.4879 (2)	0.0758 (6)
H23A	0.069174	0.272022	0.416909	0.091*
C24	0.1164 (3)	0.33910 (8)	0.50450 (17)	0.0617 (5)
H24A	0.061833	0.360817	0.445430	0.074*
C25	0.1940 (2)	0.35997 (7)	0.60985 (15)	0.0456 (4)
C26	0.2100 (4)	0.19435 (9)	0.5533 (3)	0.1151 (11)
H26A	0.268659	0.177638	0.622601	0.173*
H26B	0.091952	0.180390	0.531875	0.173*
H26C	0.276226	0.188146	0.492393	0.173*

in the expected ranges. In the crystal structure, the crystal packing is stabilized in layers and held together by van der Waals interactions.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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