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2-(Benzoylmethylsulfanyl)-6-methoxy-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.061
wR factor = 0.126
Data-to-parameter ratio = 12.7

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

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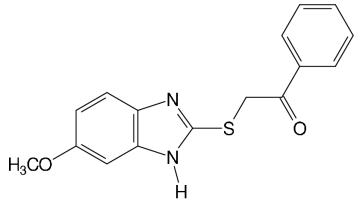
The structure of the title compound, $C_{16}H_{14}N_2O_2S$, has been determined and shows a twisted molecule with a dihedral angle of 66.31 (11) Å between the two aromatic ring systems. A single N—H···N association creates a slightly convoluted, linear hydrogen-bonded chain [graph set $C_2^2(4)$] in the *b*-axis direction.

Comment

A search of the April 2003 release of the Cambridge Structural Database (Allen, 2002) reveals that the 2-benzimidazoylthio moiety has been structurally characterized more often as a ligand in metal coordination and organometallic complexes than as a fragment of an organic compound; ratio 13:7, respectively, with four of the seven compounds being sulfinyls. As part of a series of synthetic and structural studies on *S*-substituted 2-benzimidazoylthio compounds we have characterized the structure of the title compound, (I), which shows a twisted molecule with a dihedral angle of 66.31 (11) Å between the two aromatic ring systems (Fig. 1). The assignment of N1 in the imidazoyl ring was confirmed by both the initial location of H1 in a difference syntheses and the notable differences between the N1—C2 and C2—N3 bond distances. A single N—H···N association creates a slightly convoluted, linear hydrogen-bonded chain [graph set $C_2^2(4)$] in the *b*-axis direction. Hydrogen-bonding geometry is given in Table 1.



(I)

Experimental

The title compound was obtained from Key Organics Ltd and was crystallized from ethanol.

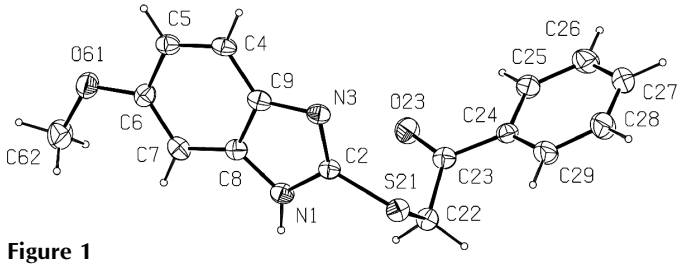


Figure 1
The molecular configuration and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$C_{16}H_{14}N_2O_2S$	D_x = 1.432 Mg m^{-3}
M_r = 298.35	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 17502 reflections
a = 5.7681 (3) Å	θ = 2.9–27.5°
b = 9.8914 (6) Å	μ = 0.24 mm^{-1}
c = 24.4281 (16) Å	T = 120 (2) K
β = 96.798 (3)°	Plate, colourless
V = 1383.94 (14) Å^3	0.26 × 0.14 × 0.02 mm
Z = 4	

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	2413 independent reflections
φ and ω scans	1676 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	R_{int} = 0.103
T_{min} = 0.941, T_{max} = 0.987	θ_{max} = 25.0°
13373 measured reflections	$h = -6 \rightarrow 6$
	$k = -11 \rightarrow 11$
	$l = -28 \rightarrow 29$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.5232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.061	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.126	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
2413 reflections	
190 parameters	
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.88	2.14	3.017 (4)	176

Symmetry code: (i) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

All H atoms were included in the refinement at calculated positions, in the riding-model approximation, with an N—H distance of 0.88 Å and C—H distances of 0.95 (aromatic H atoms), 0.99 (CH_2 H atoms) and 0.98 Å (CH_3 H atoms). The isotropic displacement parameters were set equal to $1.25U_{eq}$ of the carrier atom. The high R_{int} value for the title compound was the result of weak high-angle data.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO, SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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