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(*Z*)-4-(4-Methoxybenzylidene)-2-methylsulfanyl-3-phenethyl-1*H*-imidazol-5(4*H*)-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.05 Å
R factor = 0.082
wR factor = 0.173
Data-to-parameter ratio = 14.3

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

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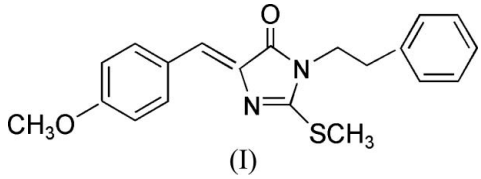
The title molecule, $C_{20}H_{20}N_2O_2S$, exits in the *Z* form and the five-membered imidazole ring and the benzene ring of the 4-methoxybenzylidene moiety are almost coplanar. Short intramolecular contacts [C···S = 3.138 (4) Å and C···N = 3.060 (4) Å] indicate the presence of weak C—H···S and C—H···N intramolecular hydrogen bonds.

Comment

Imidazolinone derivatives have been reported to possess a broad spectrum of pharmacological activities including anticonvulsant (Mehta *et al.*, 1981), antiviral (El-Barbary *et al.*, 1994) and antitumour (Khodair *et al.*, 1998) activities, and exhibit various biological properties, such as fungicidal and herbicidal activities (Yang *et al.*, 2004). The crystal structure of a closely related compound, namely (*Z*)-5-benzylidene-3-phenethyl-2-thioxoimidazolidin-4-one (Wu *et al.*, 2005), has been reported recently.



(I)

The title compound, (I), contains three essentially planar rings. The dihedral angle between the five-membered imidazolinone ring (C9/C10/C11/N1/N2) and the benzene ring of the 4-methoxybenzylidene moiety (C13–C18) is 2.60 (1)°.

Short intramolecular C···S and C···N contacts (Table 1) may indicate the presence of weak intramolecular C—H···S and C—H···N hydrogen bonds (Fig. 1). There are no significant intermolecular hydrogen-bond interactions.

Experimental

A mixture of 5-(4-methoxybenzylidene)-3-phenethyl-2-thioxoimidazol-4-one (0.77 mmol) in dry acetonitrile (40 ml), methyl iodide (1.54 mmol) and solid potassium carbonate (1.3 mmol) was stirred for 3 h at room temperature and then filtered. The filtrate was concentrated under reduced pressure, and the residue was recrystallized from dichloromethane and petroleum ether (1:4 *v*/*v*) to give the title compound in 68% yield (m.p. 402–404 K) (Yang *et al.*, 2004). Single crystals suitable for X-ray data collection were obtained by slow evaporation of an ethanol solution of (I). IR (KBr): 3021, 2927, 1698, 1637, 1595, 1500, 1452 cm^{-1}. ^1H NMR (chloroform-*d*, δ): 8.14–7.20 (*m*, 9H), 6.94 (*s*, 1H), 3.85 (*s*, 3H), 3.80 (*t*, 2H, *J* = 7.8 Hz), 2.96 (*t*, 2H, *J* = 7.8 Hz), 2.72 (*s*, 3H). ^{13}C NMR (chloroform-*d*): 169.77, 163.34, 160.94, 137.68, 136.77, 133.70, 128.84, 128.59, 127.43, 126.69, 123.94, 114.18, 55.28, 42.28, 35.01, 12.98.

Crystal data

$C_{20}H_{20}N_2O_2S$
M_r = 352.44
Triclinic, $P\overline{1}$
a = 9.7833 (10) Å
b = 9.9027 (10) Å
c = 10.2853 (11) Å
α = 101.957 (2)°
β = 104.951 (2)°
γ = 101.511 (2)°
V = 907.46 (16) Å^3
Z = 2
D_x = 1.290 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1514 reflections
θ = 2.6–24.3°
μ = 0.19 mm^{-1}
T = 298 (2) K
Block, colourless
0.27 × 0.21 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.950, T_{max} = 0.975
6756 measured reflections
3264 independent reflections
2723 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.2°
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.173
S = 1.29
3264 reflections
228 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.3033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···S1	0.97	2.74	3.138 (4)	105
C18—H18···N2	0.93	2.41	3.060 (4)	127

The H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(parent atom), and Csp^3—H = 0.96 Å with U_{iso}(H) = 1.5U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

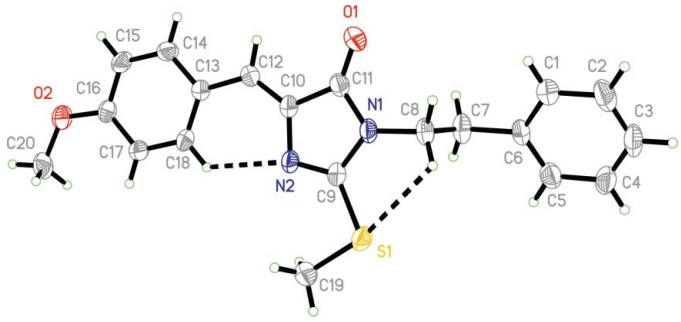


Figure 1
The formula unit of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level. Dashed lines indicate weak hydrogen-bond interactions.

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