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N-(3,5-Dimethoxybenzylidene)-2-(methylsulfanyl)aniline

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 18.0

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

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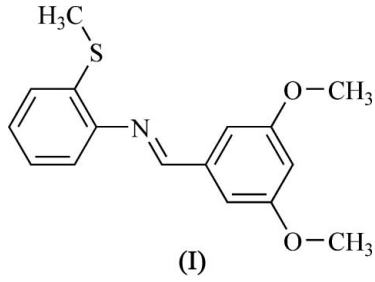
The title compound, $C_{16}H_{17}NO_2S$, has a *trans* geometry about the C=N bond. The molecule is non-planar, with a dihedral angle of 55.21 (4)° between the two aromatic rings.

Comment

Schiff base ligands are versatile ligands due to their ease of synthesis and their ability to be readily modified electronically and sterically. Schiff base ligands have been used to model enzymes (Santra *et al.*, 2002) and as supporting ligands in asymmetric catalysis (Xia *et al.*, 2005). Our group is interested in the synthesis and coordination chemistry of mixed-donor Schiff base ligands containing sulfur donors (Hamaker & Corgliano, 2006; Hamaker & Halbach, 2006; Hamaker *et al.*, 2006). As a part of our studies, we report the crystal structure of the title compound, (I).



(I)

The molecule (Fig. 1) is non-planar with a dihedral angle of 55.21 (4)° between the two aromatic rings. The C=N group is nearly coplanar with the C21–C26 ring, with an N—C20—

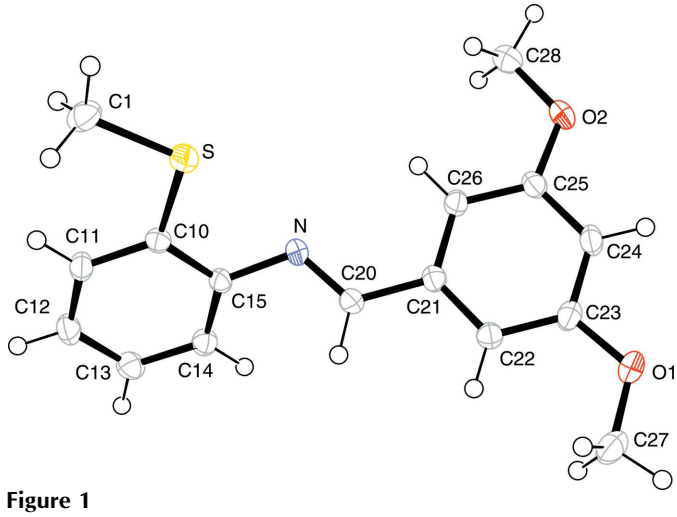


Figure 1
View of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

C21—C26 torsion angle of 171.34 (14)°. The C10–C15 ring is twisted away from the rest of the molecule due to steric repulsion between the H atoms attached to C14 and C20, with a C10—C15—N—C20 torsion angle of 137.10 (14)°. The 3,5-dimethoxybenzylidene (C20–C28/O1/O2) fragment is essentially planar, with an r.m.s. deviation of 0.0253Å. The C=N double-bond length is 1.2744 (19)Å, in agreement with values in related molecules (Hamaker & Corgliano, 2006; Hamaker *et al.*, 2006).

Experimental

Compound (I) was prepared according to the method of Hamaker & Halbach (2006). Single crystals were obtained by slow evaporation of a concentrated ethanol solution of (I).

Crystal data

$C_{16}H_{17}NO_2S$
M_r = 287.37
Monoclinic, $P2_1$
a = 7.7704 (18) Å
b = 7.8397 (9) Å
c = 12.0141 (15) Å
β = 100.230 (14)°
V = 720.2 (2) Å^3
Z = 2
D_x = 1.325 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 173 (2) K
Prism, yellow
0.48 × 0.41 × 0.35 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.900, T_{max} = 0.925
3780 measured reflections
3285 independent reflections
3185 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.05
3285 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.0994P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1518 Friedel pairs
Flack parameter: 0.02 (6)

Table 1
Selected geometric parameters (Å, °).

C15—N	1.4154 (16)	C20—N	1.2744 (19)
N—C20—C21	122.99 (13)	C20—N—C15	118.09 (12)

The H atoms were treated as riding atoms, with C—H = 0.95 (aromatic) or 0.98Å (methyl) and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms and $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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