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3-[(2-Chlorophenyl)sulfonylamino]-2-cyano-*N*-(3,5-dimethoxyphenyl)-3-methylsulfanyl-2-propenamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.087
Data-to-parameter ratio = 13.0

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

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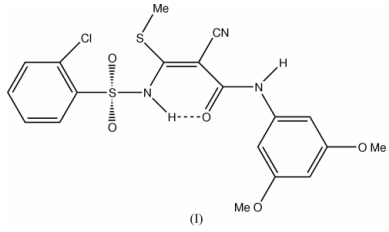
In the title compound, $C_{19}H_{18}ClN_3O_5S_2$, which is a representative of a class of inactive acetolactate synthase inhibitors, the dihedral angle between the two aromatic groups is 85.9 (1)°.

Comment

The title compound, (I), is a representative of a class of acetolactate inhibitors (McFadden *et al.*, 1993). The present paper reports the relevant bond distances and angles for this compound.



(I)

The C3—C31 bond length of 1.430 (3) Å is much longer than expected for a Csp^2—Csp bond (Fig. 1 and Table 1). A general survey of this type of bond (S)(N)C═C(C)—CN using well determined structures from the Cambridge Structural Database (September 2002 update; Allen, 2002) gave a mean of 1.43 (1) Å. This search was restricted to compounds with available coordinates, no disorder, no polymers, R < 0.10, and error-free. The dihedral angle between the two aromatic groups is 85.9 (1)°. There is an intramolecular N5—H5···O21 hydrogen bond (Table 2).

Experimental

The synthesis of (I) has been reported by McFadden *et al.* (1993).

Crystal data

$C_{19}H_{18}ClN_3O_5S_2$
M_r = 467.16
Triclinic, $P\overline{1}$
a = 9.506 (1) Å
b = 9.738 (2) Å
c = 12.572 (2) Å
α = 109.65 (1)°
β = 94.14 (1)°
γ = 106.24 (1)°
V = 1034.3 (3) Å^3
Z = 2
D_x = 1.502 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–12°
μ = 0.42 mm^{-1}
T = 293 (2) K
Needle, colourless
0.30 × 0.05 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.958, T_{max} = 0.980
3933 measured reflections
3639 independent reflections
3027 reflections with $I > 2\sigma(I)$
R_{int} = 0.006
θ_{max} = 25.0°
$h = 0 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.4158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.030$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.087$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.32$ e Å^{-3}
3639 reflections	
279 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C2—C3	1.483 (2)	C3—C31	1.430 (3)
C3—C4	1.371 (2)	C31—N32	1.139 (2)
C12—C11—N1—C2	2.6 (3)	C3—C4—N5—S6	170.64 (15)
C11—N1—C2—C3	177.31 (17)	C4—N5—S6—C61	−57.85 (19)
N1—C2—C3—C4	−179.67 (17)	N5—S6—C61—C62	−54.47 (18)
C2—C3—C4—N5	−3.9 (3)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O21	0.85	1.92	2.599 (2)	135

Data collection: *Data Collection Package* (Frenz & Enraf–Nonius, 1985); cell refinement: *Data Collection Package*; data reduction: *WinGX* (Version 1.64.02; Farrugia, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*98 (Spek, 1988); software used to prepare material for publication: *SHELXL*97.

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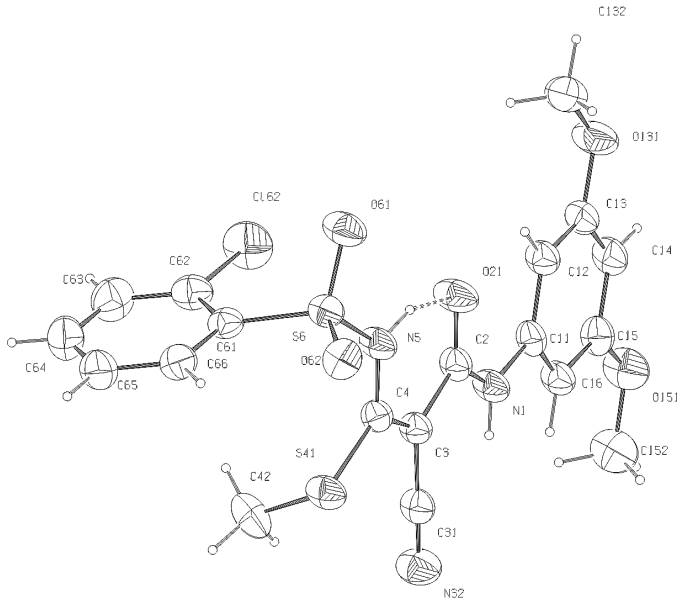

Figure 1
Molecular structure of the title compound, (I), with displacement ellipsoids drawn at the 50% probability level.

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