

(Z)-3-(4-Chlorophenyl)-2-[[N-(2-formylphenyl)-4-methylbenzenesulfonamido]-methyl]prop-2-enitrile

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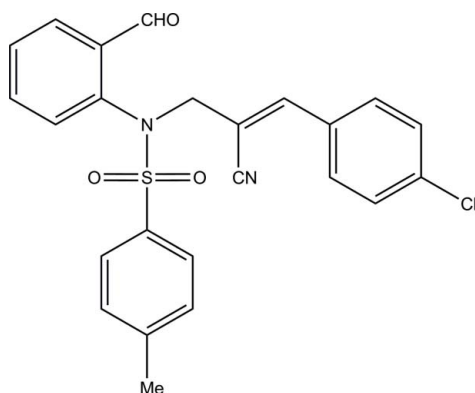
Received 1 December 2011; accepted 5 December 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 17.3.

In the title compound, $\text{C}_{24}\text{H}_{19}\text{ClN}_2\text{O}_3\text{S}$, the sulfonyl-bound benzene ring forms dihedral angles of 38.1 (2) and 81.2 (1)°, respectively, with the formyl benzene and benzene rings. The molecular conformation is stabilized by a weak intramolecular C—H···O hydrogen bond, which generates an S(5) ring motif. The crystal packing is stabilized by C—H···O hydrogen bonds, which generate C(7) zigzag chains along [010] and R₃²(19) ring motifs along [010]. The crystal packing is further stabilized by C—Cl··· π interactions [Cl···centroid = 3.456 (2) Å and C—Cl···centroid = 173.4 (2)°].

Related literature

For background to the pharmacological uses of sulfonamides, see: Korolkovas (1988); Mandell & Sande (1992). For related structures, see: Ranjith *et al.* (2009); Aziz-ur-Rehman *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



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Experimental

Crystal data

$\text{C}_{24}\text{H}_{19}\text{ClN}_2\text{O}_3\text{S}$
 $M_r = 450.92$
 Orthorhombic, $P2_12_12_1$
 $a = 8.9795 (5) \text{ \AA}$
 $b = 10.1590 (5) \text{ \AA}$
 $c = 25.1050 (13) \text{ \AA}$
 $V = 2290.1 (2) \text{ \AA}^3$
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.29 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 $0.25 \times 0.23 \times 0.17 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.931, T_{\text{max}} = 0.953$
 12721 measured reflections
 4850 independent reflections
 3396 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.111$
 $S = 1.03$
 4850 reflections
 281 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983),
 2049 Friedel pairs
 Flack parameter: 0.06 (8)

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···O3	0.97	2.43	2.890 (3)	109
C3—H3···O2 ⁱ	0.93	2.57	3.345 (3)	141
C15—H15A···O2 ⁱⁱ	0.97	2.57	3.385 (3)	142
C23—H23···O1 ⁱⁱⁱ	0.93	2.45	3.114 (4)	128

Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, y + 1, z$.

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT (Bruker, 2004); data reduction: SAINT and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

The authors thank Dr Babu Vargheese, SAIF, IIT, Madras, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5740).

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