organic papers

2-(4-Bromophenyl)-3,3-bis(methylsulfanyl)-prop-2-enenitrile

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Key indicators

Single-crystal X-ray study
$T = 294$ K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.145
Data-to-parameter ratio = 15.9

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

In the title compound, $C_{11}H_{10}BrNS_2$, the molecules are linked into sheets stabilized by C—H⋯N, C—Br⋯Br and C—S⋯Br short contacts.

Comment

The title compound, (I) (Fig. 1), is an intermediate in the synthesis of heterocyclic ketene aminals which are powerful and versatile intermediates for the synthesis of a wide variety of fused hetereocylic compounds (Wang & Huang, 2002).
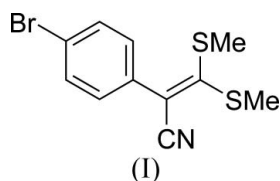
In (I), the bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The C7—C9 bond [1.343 (7) Å] is shorter than the C7—C8 [1.443 (7) Å] and C6—C7 [1.479 (7) Å] bonds, indicating its double-bond nature. The shortening of bonds C9—S1 [1.743 (5) Å] and C9—S2 [1.764 (5) Å] with respect to bonds C10—S1 [1.809 (6) Å] and C11—S2 [1.808 (6) Å] is attributed to d–π interactions between sulfur and the olefin.

In the packing of the title compound, there is one intermolecular C5–H5⋯N1^i hydrogen bond [H5⋯N1^i = 2.69 Å, C5⋯N1^i = 3.379 (7) Å and C5—H5⋯N1^i = 131°; symmetry code: (i) $1 - x$, $-\frac{1}{2} + y$, $\frac{1}{2} - z$], one intermolecular C3—Br⋯Br^{ii} short contact [Br⋯Br^{ii} = 3.515 (3) Å, C3⋯Br^{ii} =
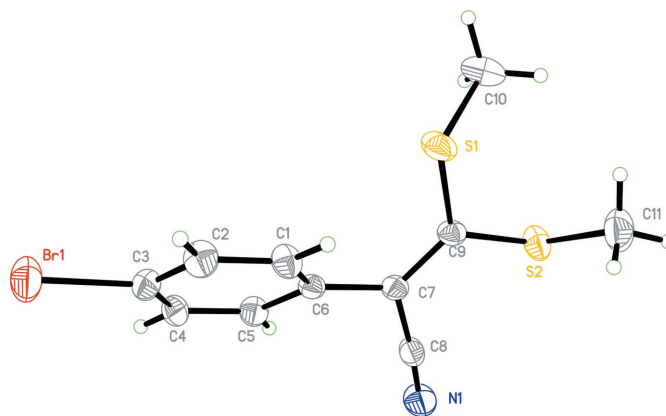

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

5.402 (7) Å and C3···Br···Br^{ii} = 168 (2)°; symmetry code: (ii) $1 - x, -1 - y, 1 - z$] and an intermolecular C9—S1···Br short contact [S1···Br = 3.684 (3) Å, C9···Br = 5.400 (6) Å and C9–Br···Br = 168 (2)°] (Fig. 2).

Experimental

The title compound, (I), was prepared according to the procedure of Liljefors & Sandström (1970). Suitable crystals were obtained by evaporation of an acetone solution (m.p. 346 K).

Crystal data

$C_{11}H_{10}BrNS_2$	$Z = 4$
$M_r = 300.23$	$D_x = 1.596$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.558$ (10) Å	$\mu = 3.59$ mm^{-1}
$b = 7.285$ (9) Å	$T = 294$ (2) K
$c = 20.04$ (2) Å	Block, colorless
$\beta = 90.010$ (8)°	$0.20 \times 0.18 \times 0.12$ mm
$V = 1249$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	6007 measured reflections
	2196 independent reflections
φ and ω scans	1543 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.065$
$T_{min} = 0.534$, $T_{max} = 0.673$	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$+ 1.8209P]$
$wR(F^2) = 0.145$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
2196 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
138 parameters	$\Delta\rho_{min} = -0.85$ e Å^{-3}
H-atom parameters constrained	

H atoms were constrained to idealized geometry using a riding model; $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H = 0.95 (CH group) or 0.99 Å (CH$_2$ groups), with $U_{iso}(H) = 1.2$ (aromatic C) or 1.5 (methyl C) times $U_{eq}(C)$.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics:
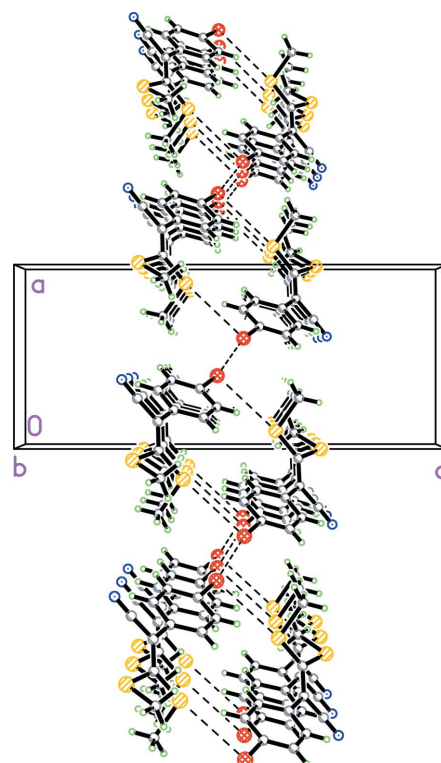

Figure 2
The packing of (I). The dotted lines indicate Br···Br and S···Br short contacts.

SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

References

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