

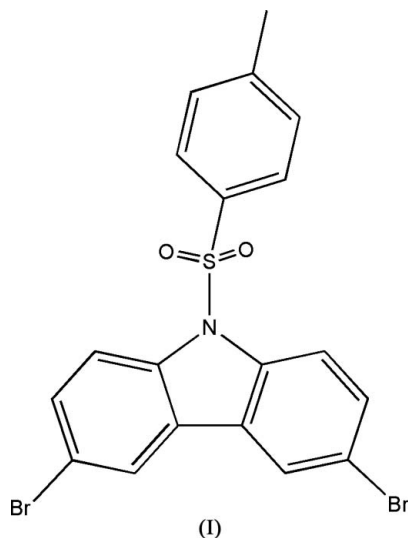
## 3,6-Dibromo-9-(4-tolylsulfonyl)-9H-carbazole

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## Key indicators

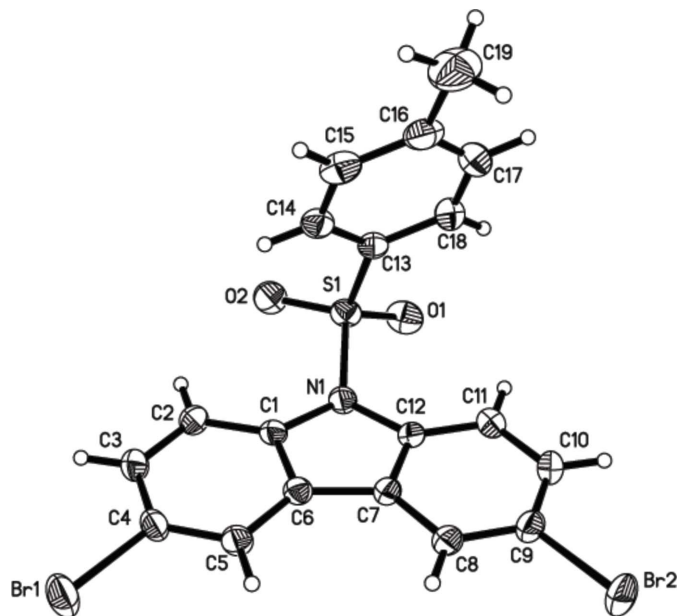
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.112  
Data-to-parameter ratio = 16.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The title compound,  $\text{C}_{19}\text{H}_{13}\text{Br}_2\text{NO}_2\text{S}$ , was synthesized by *N*-alkylation of 4-methylbenzenesulfonyl chloride with 3,6-dibromo-9H-carbazole. The carbazole ring system is essentially planar, with a mean deviation of 0.024 Å, and makes a dihedral angle of 75.46 (9)° with the plane of the benzene ring.Received 16 March 2006  
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## Comment

Carbazole derivatives substituted by *N*-alkylation show useful pharmaceutical properties (Buu-Hoi & Royer, 1950; Harfenist & Joyner, 1983; Caulfield *et al.*, 2002; Harper *et al.*, 2002). This paper reports the structure of 3,6-dibromo-9-(4-tolylsulfonyl)-9H-carbazole, (I), which was synthesized by *N*-alkylation of 4-methylbenzenesulfonyl chloride with 3,6-dibromo-9H-carbazole.The carbazole ring system is essentially planar, with a mean deviation of 0.024 Å. The dihedral angle formed between the carbazole ring system and the plane of the benzene ring is 75.46 (1)°. The C—Br distances are 1.915 (4) and 1.916 (4) Å, consistent with literature values (Allen *et al.*, 1987).

## Experimental

The title compound, (I), was prepared according to the procedure of Chakrabarti *et al.* (1989). 3,6-Dibromo-9H-carbazole (1.95 g) (Smith *et al.*, 1992) in a solution of dimethylformamide (25 ml) and benzene (25 ml) was treated with sodium hydride (0.168 g) in an ice bath for 30 min. To the cold stirred solution, 4-methylbenzenesulfonyl chloride (1.12 g) was added and the mixture stirred at room temperature for a further 4 h. The resulting mixture was then poured into water (40 ml) and extracted with benzene (100 ml). After drying



**Figure 1**  
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

the benzene extracts over anhydrous sodium sulfate, filtration and concentration, the solid product was recrystallized from EtOH, giving crystals of (I) (yield: 1.36 g, 98%; m.p. 494 K). Compound (I) (40 mg) was dissolved in a mixture of chloroform (6 ml) and ethanol (2 ml), and the solution was kept at room temperature for 10 d. Natural evaporation of the solution gave colourless crystals suitable for X-ray analysis.

*Crystal data*

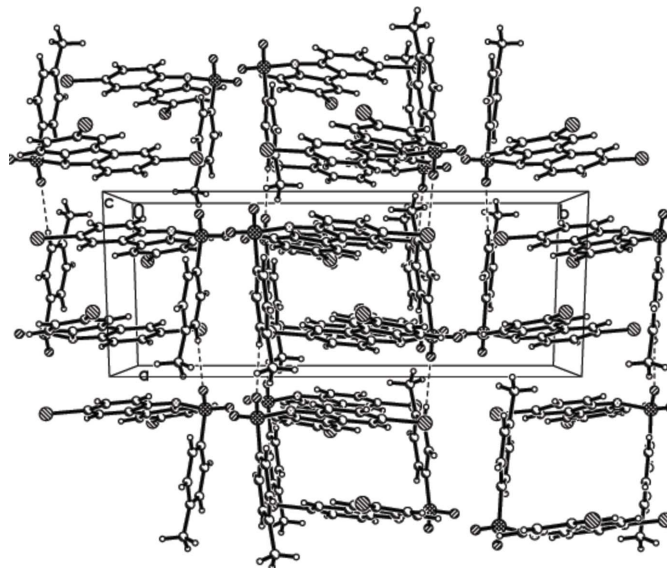
C<sub>19</sub>H<sub>13</sub>Br<sub>2</sub>NO<sub>2</sub>S  
*M<sub>r</sub>* = 479.18  
 Monoclinic, *P*<sub>2</sub><sub>1</sub>/*c*  
*a* = 8.312 (4) Å  
*b* = 20.573 (11) Å  
*c* = 11.374 (6) Å  
 β = 106.867 (9)°  
*V* = 1861.3 (16) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.710 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 μ = 4.48 mm<sup>-1</sup>  
*T* = 294 (2) K  
 Block, colourless  
 0.24 × 0.20 × 0.14 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer  
 φ and ω scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1997)  
*T<sub>min</sub>* = 0.413, *T<sub>max</sub>* = 0.573 (expected range = 0.385–0.534)  
 10105 measured reflections  
 3733 independent reflections  
 2508 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.047  
*θ<sub>max</sub>* = 26.4°

*Refinement*

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.043  
*wR*(*F*<sup>2</sup>) = 0.113  
*S* = 1.04  
 3733 reflections  
 227 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.1434P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 (Δ/*σ*)<sub>max</sub> = 0.003  
 Δρ<sub>max</sub> = 0.67 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.65 e Å<sup>-3</sup>



**Figure 2**  
Part of the packing of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C15—H15···O1 <sup>i</sup>	0.93	2.54	3.450 (6)	166

Symmetry code: (i) *x* + 1, *y*, *z*.

All H atoms were included in the riding model approximation, with C—H = 0.93 (aromatic) and 0.96 Å (methyl), and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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, 1997); software used to prepare material for publication: SHELXTL.

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