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[5-Fluoro-2-(4-iodo-2-nitrophenylsulfanyl)-phenyl]-*N*,*N*-dimethylmethanamine

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Key indicators

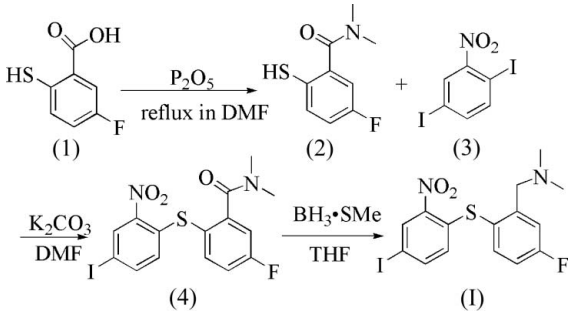
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.057
Data-to-parameter ratio = 14.2

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

In the title compound, two aromatic rings are almost perpendicular to each other with a dihedral angle of 72.4 (1)°.

Comment

Alterations in serotonergic neuronal function, particularly changes in serotonin transporter (SERT) densities, occur in a large number of neuropsychiatric disorders (Brust *et al.*, 2006). Imaging of SERT with positron emission tomography (PET) and single photon emission computed tomography (SPECT) in humans could provide a useful tool for understanding how alterations of this system are related to depressive illnesses and other psychiatric disorders, as well as monitoring the treatment of depressed patients. In the past few years, a series of diphenyl sulfides have emerged as selective SERT imaging agents (Jarkas *et al.*, 2005; Huang *et al.*, 2005; Emond *et al.*, 2002; Wilson *et al.*, 2000). The three-dimensional quantitative structure–activity relationship (three-dimensional QSAR) of the diphenyl sulfide analogues will help us understand the nature of the interaction between the SERT ligands and the SERT; in this context it is important to obtain crystal structural data for the analogues.



The molecular structure of (I) is shown in Fig. 1. The two aromatic rings are almost perpendicular with a dihedral angle of 72.4 (1)°. The dihedral angle between the plane of the nitro group and the attached aromatic ring is 13.9 (1)°. The *N*,*N*-dimethylaminomethyl group can be viewed as a trigonal pyramidal framework.

Experimental

The title compound, (I), was synthesised according to the literature method of Oya *et al.* (2000) (see scheme above). Briefly, 1,4-diiodo-2-nitrobenzene was coupled with 5-fluoro-2-mercapto-*N*,*N*-dimethylbenzamide in DMF to afford compound (4), which was reduced with BH_3–SMe_2 complex to give compound (I). Single crystals suitable for X-ray diffraction analysis, were obtained by slow evaporation of an acetone solution.

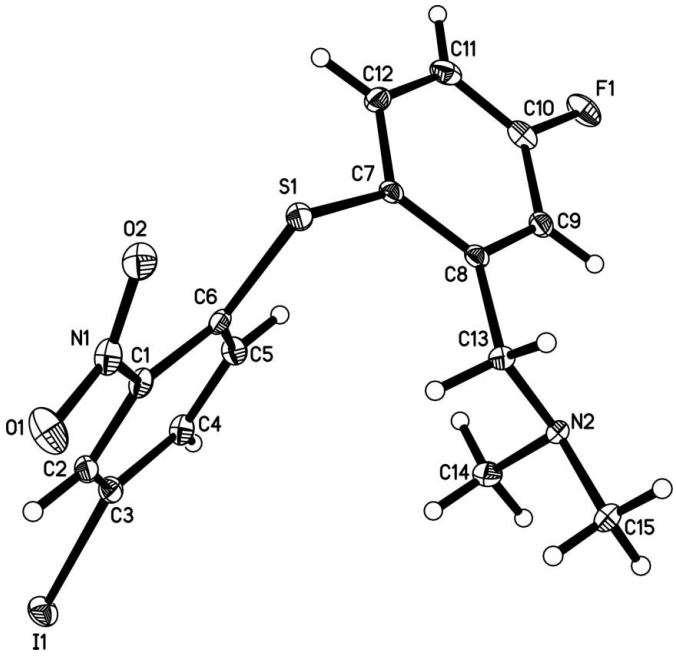


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

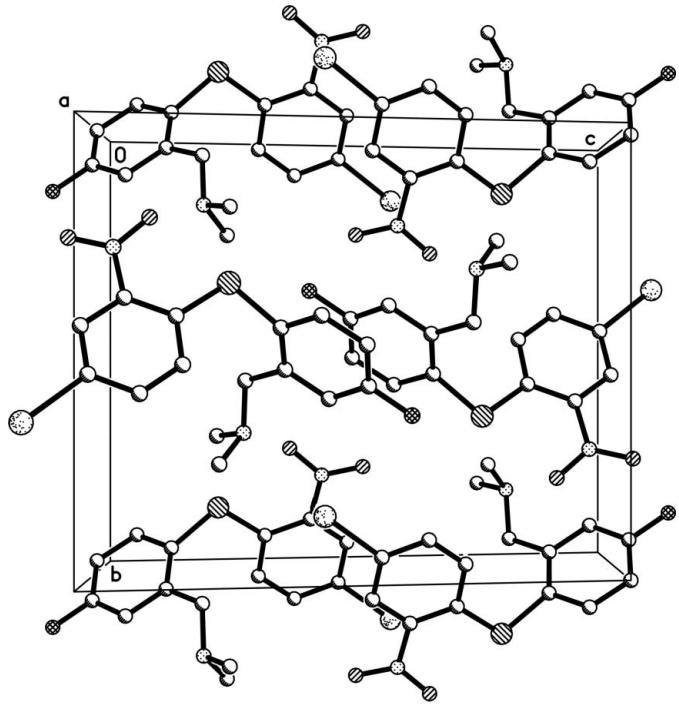


Figure 2
The crystal packing of (I), viewed along the *a* axis. H atoms have been omitted.

Crystal data

$C_{15}H_{14}FIN_2O_2S$
M_r = 432.24
Monoclinic, $P2_1/c$
a = 8.7213 (17) Å
b = 12.530 (3) Å
c = 15.135 (3) Å
β = 101.29 (3)°
V = 1622.0 (6) Å^3
Z = 4
D_x = 1.770 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.12 mm^{-1}
T = 293 (2) K
Block, colorless
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.653, T_{max} = 0.728
9624 measured reflections
2859 independent reflections
2586 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.057
S = 1.06
2859 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl 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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