Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[4-(2,3-Dichlorophenyl)piperazin-1-yl][2-(2-methoxyphenylsulfanyl)phenyl]methanone

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.107
Data-to-parameter ratio = 16.3

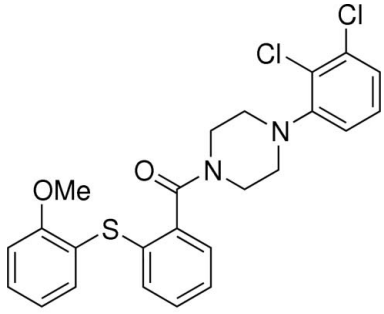
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 January 2006
Accepted 8 February 2006

In the title compound, $C_{24}H_{22}Cl_2N_2O_2S$, synthesized from 2-(2-methoxyphenylsulfanyl)benzoyl chloride and 1-(2,3-dichlorophenyl)piperazine, the piperazine ring adopts a normal chair conformation.

Comment

Substituted diphenyl sulfide derivatives which display high *in vitro* and *in vivo* affinities for serotonin transporter (SERT), high selectivity for the dopamine transporter (DAT) and partial selectivity for norepinephrine transporter sites (NET) have been described as potent and selective SERT ligands (Mehta & Brieaddy, 1997; Wilson & Houle, 1999; Younes *et al.*, 2000).



(I)

The structure of (I) is illustrated in Fig. 1. The piperazine ring has a normal chair conformation. The dihedral angle relating the two rings bonded to the S atom is 102.28 (12)°. The dichlorophenyl ring is also twisted with respect to the piperazine ring [C19—N2—C17—C18 = 164.8 (2)°].

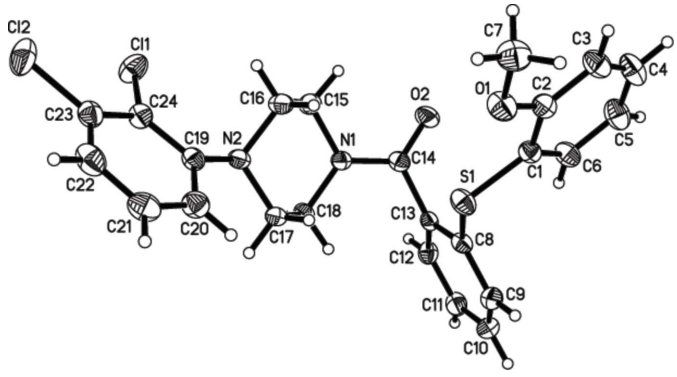


Figure 1
The molecular structure of (I), drawn with 30% probability ellipsoids.

Experimental

2-(2-Methoxyphenylsulfanyl)benzoyl chloride (8 mmol), triethylamine (20 mmol) and 1-(2,3-dichlorophenyl)piperazine (8 mmol) in $CHCl_3$ (60 ml) were stirred at room temperature for 3 h. The mixture was then washed with 2 *M* sodium hydroxide. The organic layer was dried and evaporated *in vacuo* to dryness, giving a yellow oil, which solidified at room temperature. After filtration through active charcoal and recrystallization from 60% aqueous ethanol (70 ml), the title compound was obtained as white crystals. Crystals suitable for X-ray analysis were grown by slow evaporation of an absolute methanol solution at room temperature over a period of 15 d.

Crystal data

$C_{24}H_{22}Cl_2N_2O_2S$
M_r = 473.40
Monoclinic, $P2_1/c$
a = 17.034 (3) Å
b = 7.6898 (14) Å
c = 17.229 (3) Å
β = 99.344 (3)°
V = 2226.9 (7) Å^3
Z = 4
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2087 reflections
θ = 2.4–21.9°
μ = 0.41 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.900, T_{max} = 0.921
12169 measured reflections
4587 independent reflections
2529 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 26.5°
$h = -21 \rightarrow 19$
$k = -7 \rightarrow 9$
$l = -21 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.107
S = 0.99
4587 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.1467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

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*.

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Mehta, N. B. & Brieaddy, L. E. (1997). US Patent No. 4 056 632.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wilson, A. A. & Houle, S. (1999). *J. Labelled Compd Radiopharm.* **42**, 1277–1288.
Younes, S., Labssita, Y., Baziard-Mouysset, G., Payard, M., Rettotri, M. C., Renard, P., Pfeiffer, B., Caiqnard, D. H. (2000). *Eur. J. Med. Chem.* **35**, 107–121.