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N-[(4-Methylphenyl)sulfanyl]phthalimide

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Key indicators

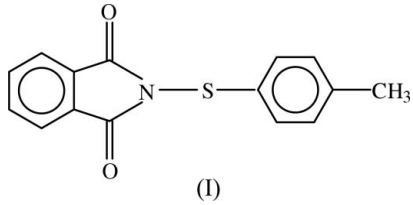
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.109
Data-to-parameter ratio = 17.3

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

In the title compound, $C_{15}H_{11}NO_2S$, the dihedral angle between the two planar ring systems is 74.49 (5)°.

Comment

Phthalimides exhibit various biological properties and have been reported as antipsychotics (Norman *et al.*, 1996), anti-inflammatory agents (Collin *et al.*, 2001) and herbicides (Kawaguchi & Ilkeda, 2001).



(I)

In the title compound, (I), the pair of torsion angles from the imide N atom to the *p*-methylphenylthio ring are N1—S1—C9—C10 = − 98.24 (15)° and N1—S1—C9—C14 = 83.73 (14)°. The angle C9—S1—N1 is 101.59 (7)°. As a result, the molecule exhibits a roof-shaped conformation. The phthalimide ring system is essentially planar and is twisted with respect to the *p*-methylphenylthio ring with a dihedral angle of 74.49 (5)°. The phthalimide ring systems interact in pairs *via* π–π stacking interactions. In these pairs, the distance between the centre of the six-membered ring of one molecule and the centre of the five-membered ring of another molecule is 3.539 (11) Å (symmetry code for the second molecule: 1 − *x*, 1 − *y*, 1 − *z*). There is also a C—H···π interaction between the *p*-methylphenyl ring and atom H4 of the phthalimide ring. The distance between atom H4 bonded to atom C4 and the ring centroid is 2.936 Å (symmetry code: 2 − *x*, 1 − *y*, 1 − *z*) and the C4—H4···centroid angle is 146.9° (Fig. 2).

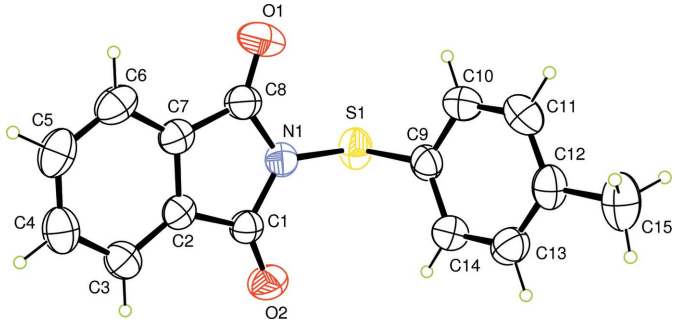


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids.

Experimental

4-Methylbenzenethiol (15.19 g, 0.105 mol) and phthalimide (14.70 g, 0.10 mol) were dissolved in hot pyridine (40 ml) and acetonitrile (50 ml), and the stirred solution was cooled to room temperature. A solution of bromine (19.2 g, 6.19 ml, 0.12 mol) in acetonitrile (50 ml) was then added dropwise over 30 min. After a further period of 2 h, methanol (200 ml) was added dropwise over 30 min. The products were cooled (ice–water) for 30 min, and then filtered to give the title compound as yellow crystals (yield 14.55 g, 89%, m.p: 471–476 K).

Crystal data

$C_{15}H_{11}NO_2S$
M_r = 269.31
Triclinic, $P\overline{1}$
a = 7.2186 (8) Å
b = 8.3180 (10) Å
c = 11.5374 (13) Å
α = 103.142 (10)°
β = 99.418 (9)°
γ = 101.976 (9)°
V = 643.57 (13) Å^3
Z = 2
D_x = 1.390 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 296 K
Plate, yellow
0.75 × 0.51 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.826, T_{max} = 0.980
9810 measured reflections
2979 independent reflections
2533 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 27.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.109
S = 1.02
2979 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1565P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

H atoms were placed in calculated positions and refined using a riding model, with aromatic C—H = 0.93 and methyl C—H = 0.96 Å, with U_{iso}(H) values set at 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

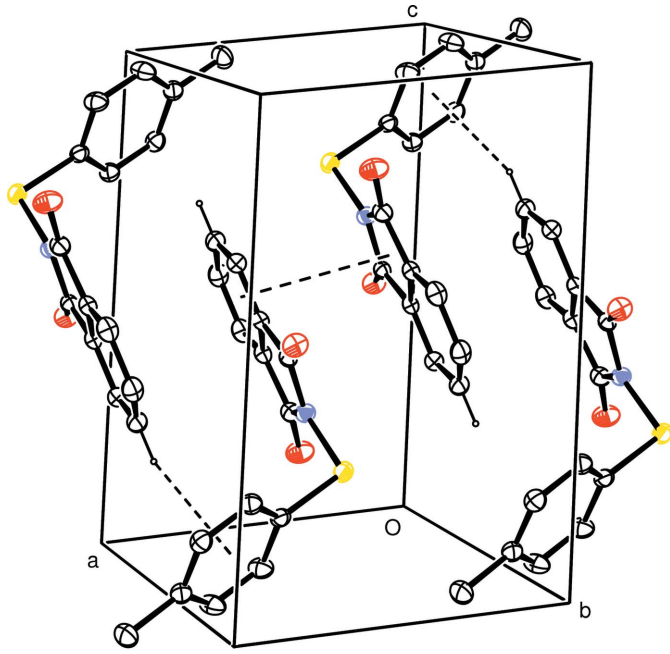


Figure 2
A packing diagram of the title compound. C—H···π hydrogen bonds and π–π interactions are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

References

Collin, X., Robert, J.-M., Wielgosz, G., Le Baut, G., Bobin- Dubigeon, C., Grimaud, N. & Petit, J.-Y. (2001). *Eur. J. Med. Chem.* **36**, 639–649.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kawaguchi, S. & Ilkeda, O. (2001). Jpn Patent Appl. JP 2001 328 911.
Norman, M. H., Minick, D. J. & Rigdon, G. C. (1996). *J. Med. Chem.* **39**, 149–157.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.