Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(*p*-Methoxyphenylsulfanyl)phthalimide

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Received 16 January 2007
Accepted 17 January 2007

In the molecule of the title compound, $C_{15}H_{11}NO_3S$, the dihedral angle between the phthalimide ring system and the benzene ring is 74.07 (8)°.

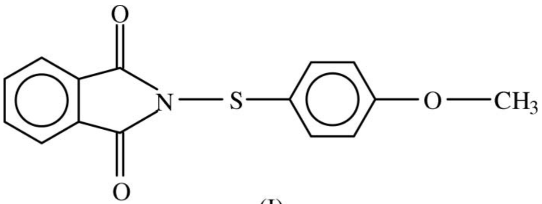
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.105
Data-to-parameter ratio = 17.6

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

Comment

Phthalimide derivatives substituted by *N*-alkylation exhibit useful pharmaceutical properties (Chapman *et al.*, 1983; Donahoe *et al.*, 1957). In the title comound, (I), the dihedral angle between the phthalimide ring system and the benzene ring is 74.07 (8)°. There are no classical hydrogen bonds, just two weak C—H···O contacts (Table 1).



(I)

Experimental

4-Methoxybenzenethiol (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 a period of 30 min. After a further 2 h, methanol (200 ml) was added dropwise over a period of 30 min. The products were cooled (ice–water bath) for 30 min, and then filtered to give (I) as yellow crystals (yield 11.70 g, 76%; m.p 475.0–477.5 K).

Crystal data

$C_{15}H_{11}NO_3S$
M_r = 285.31
Triclinic, $P\overline{1}$
a = 8.2600 (9) Å
b = 8.4479 (10) Å
c = 11.4776 (13) Å
α = 109.586 (9)°
β = 93.093 (9)°
γ = 112.998 (9)°
V = 678.61 (13) Å^3
Z = 2
D_x = 1.396 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 293 (2) K
Plate, yellow
0.68 × 0.38 × 0.03 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min}$ = 0.895, $T_{\max}$ = 0.990
10429 measured reflections
3185 independent reflections
2443 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
$\theta_{\max}$ = 27.8°

doi:10.1107/S1600536807002541

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.105$
$S = 1.04$
3185 reflections
181 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 0.1535P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.93	2.42	3.332 (3)	168
C15—H15*B*···O1^{ii}	0.96	2.49	3.428 (3)	166

Symmetry codes: (i) *x*, *y* − 1, *z*; (ii) *x* − 1, *y*, *z*.

H atoms were included in calculated positions and refined using a riding model, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å. U_{iso}(H) values were 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).

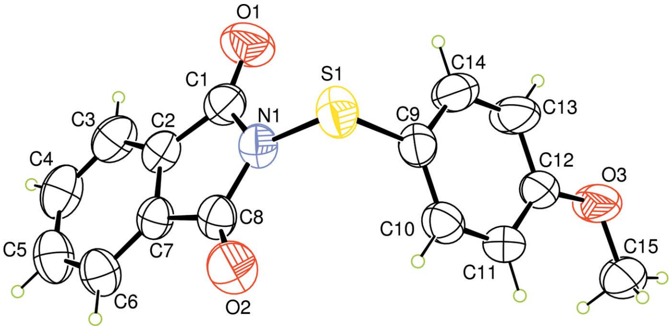


Figure 1
The molecular structure of the title compound, shown with 50% probability displacement ellipsoids.

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