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N,*N*′-Bis(phenylcarbamothioyl)benzene-1,3-dicarboxamide

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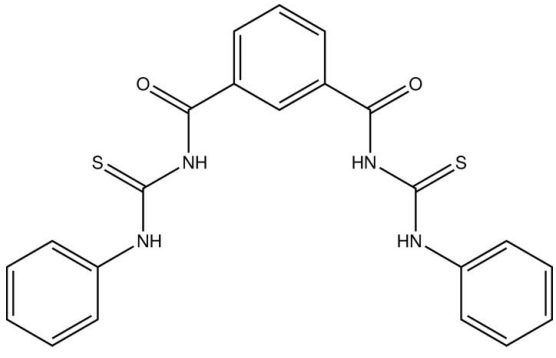
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 25.4.

The asymmetric unit of the title compound, $C_{22}H_{18}N_4O_2S_2$, contains two molecules. In one of them, the dihedral angles between the central benzene ring and the phenyl rings are 16.97 (8) and 20.97 (8)°, while the phenyl rings make a dihedral angle of 37.87 (8)°. In the other molecule, the corresponding values are 34.92 (7), 53.90 (7) and 60.68 (8)°, respectively. In each molecule, two intramolecular N—H···O hydrogen bonds generate S(6) rings and a short C—H···S contact also occurs. In the crystal, N—H···S, N—H···O, C—H···O and C—H···S interactions link the molecules into a three-dimensional network.

Related literature

For biological applications of benzimidazole derivatives, see: Madan *et al.* (1991); Fernandez *et al.* (2005); Kucukguzel *et al.* (2008); Saeed *et al.* (2009). For biological properties of thioureas, see: Rauf *et al.* (2009).



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Experimental

Crystal data

$C_{22}H_{18}N_4O_2S_2$
M_r = 434.52
Triclinic, $P\overline{1}$
a = 11.1812 (2) Å
b = 11.5623 (2) Å
c = 16.4471 (2) Å
α = 101.420 (1)°
β = 98.127 (1)°
γ = 101.316 (1)°
V = 2007.43 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 100 K
0.47 × 0.33 × 0.11 mm

Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.876, T_{max} = 0.968
41276 measured reflections
14580 independent reflections
11642 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.03
14580 reflections
573 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1NA···O1A	0.83 (2)	1.976 (19)	2.6722 (16)	140.9 (19)
N2A—H2NA···S2B^{i}	0.85 (2)	2.59 (2)	3.4201 (12)	165.0 (19)
N3A—H3NA···O2B^{ii}	0.864 (19)	2.31 (2)	2.9715 (15)	133.3 (18)
N4A—H4NA···O2A	0.90 (2)	1.86 (2)	2.6064 (17)	138.2 (18)
N1B—H1NB···O1B	0.86 (2)	1.88 (2)	2.6248 (17)	144.5 (19)
N2B—H2NB···S1B^{iii}	0.834 (19)	2.71 (2)	3.4961 (12)	158.3 (19)
N3B—H3NB···S1A^{i}	0.84 (2)	2.62 (2)	3.4336 (12)	163.0 (18)
N4B—H4NB···O2B	0.87 (2)	1.92 (2)	2.6543 (16)	141.1 (19)
C5A—H5AA···S1A	0.95	2.51	3.1910 (16)	129
C1B—H1BA···S1B	0.95	2.68	3.2693 (15)	121
C4B—H4BA···O2A^{iv}	0.95	2.55	3.4819 (18)	165
C10B—H10B···S2A^{v}	0.95	2.84	3.4570 (15)	123
C11B—H11B···S2A^{v}	0.95	2.85	3.4687 (15)	123
C14A—H14A···O2B^{ii}	0.95	2.35	3.2700 (17)	164
C14B—H14B···O1A^{ii}	0.95	2.36	3.2897 (17)	165

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+1, -z$; (iv) $-x+1, -y+1, -z+1$; (v) $x-1, y+1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7103).