4-(3-Methyl-4,5-dihydro-1H-benzo[g]-indazol-1-yl)benzenesulfonamide

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Key indicators: single-crystal X-ray study; T = 100 K; mean |C–C| = 0.005 Å; R factor = 0.068; wR factor = 0.184; data-to-parameter ratio = 14.4.

In the title compound, C18H17N3O2S, the aromatic ring bearing the sulfamide unit is aligned at 61.65 (1)° with respect to the pyrrole ring; its amino group forms N—H···N and N—H···O hydrogen bonds to neighboring molecules, generating sheets in the ac plane.

Related literature

For the crystal structure of a pyrrole synthesized using 2-acetyltetralone as a reactant, see: Portilla et al. (2007).

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2010)
Tmin = 0.600, Tmax = 0.703

Refinement

R[F2 > 2σ(F2)] = 0.068
wR(F2) = 0.184
S = 1.11
3255 reflections
226 parameters
14 restraints

H atoms treated by a mixture of independent and constrained refinement
Δρmax = 0.70 e Å−3
Δρmin = −0.65 e Å−3

Table 1

Hydrogen-bond geometry (Å, °).

Symmetry codes: (i) x+1/2, y+1/2, z; (ii) x−1, y, z.

Table 2

Experimental

Crystal data

C18H17N3O2S
Mr = 339.41
Monoclinic, P21/n
a = 4.8838 (1) Å
b = 27.3894 (4) Å
c = 12.2399 (2) Å
β = 94.738 (1)°
V = 1631.67 (5) Å³
Z = 4
Cu Kα radiation
μ = 1.89 mm−1
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

11808 measured reflections
3255 independent reflections
3166 reflections with I > 2σ(I)
Rint = 0.018

Refinement

R[F2] = 0.068
wR(F2) = 0.184
S = 1.11
3255 reflections
226 parameters
14 restraints

H atoms treated by a mixture of independent and constrained refinement
Δρmax = 0.70 e Å−3
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Table 1

Hydrogen-bond geometry (Å, °).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5614).

References


