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5-Hydroxy-3-phenyl-5-trifluoromethyl-4,5-dihydro-1*H*-pyrazole

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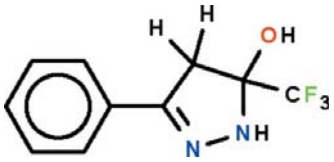
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.087; data-to-parameter ratio = 8.0.

The five-membered dihydropyrazole ring in the title compound, $C_{10}H_9F_3N_2O$, is approximately planar (r.m.s. deviation 0.111 Å for all non-H atoms) and its phenyl substituent is aligned at an angle of 14.7 (2)°. Adjacent molecules are linked by N—H···O and O—H···N hydrogen bonds, generating ribbons running along the b axis of the monoclinic unit cell.

Related literature

For the synthesis, see: Yakimovich *et al.* (2002); Zelenin *et al.* (1995). For two related structures, see: Dias & Goh (2004); Yang & Raptis (2003).



Experimental

Crystal data

$C_{10}H_9F_3N_2O$
M_r = 230.19
Monoclinic, $P2_1$
a = 9.1000 (6) Å
b = 5.4032 (3) Å
c = 10.4515 (7) Å
β = 108.139 (7)°
V = 488.35 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 100 K
0.20 × 0.15 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.972, T_{max} = 0.986
4222 measured reflections
1230 independent reflections
1060 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 1.05
1230 reflections
153 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.84 (1)	2.03 (2)	2.833 (3)	162 (4)
N2—H2···O1^{ii}	0.88 (1)	2.13 (2)	2.974 (3)	161 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, y+\frac{1}{2}, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5617).

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