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5-(4-Hexyl-1*H*-1,2,3-triazol-1-yl)-2,1,3-benzoxadiazole

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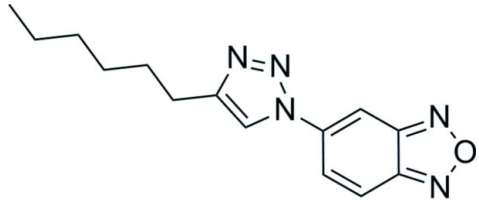
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 17.2.

The title compound, $C_{14}H_{17}N_5O$, a 1,2,3-triazole derivative of benzoxadiazole ($C_{14}H_{17}N_5O$), was synthesized *via* Cu-catalysed azide–alkyne cycloaddition (CuAAC) from the corresponding *n*-octyne and 4-azidobenzoxadiazole. The benzoxadiazole and triazole rings show a roughly planar orientation [dihedral angle between the ring planes = 12.18 (5)°]. The alkane chain adopts a zigzag conformation, which deviates from the central triazole ring by 20.89 (6)°. These two torsion angles result in an overall twist to the structure, with a dihedral angle of 32.86 (7)° between the benzoxadiazole group and the hexyl chain. The crystal structure features C—H···N hydrogen bonds leading to chains propagating along [2$\bar{1}$0] and offset parallel stacking interactions of the triazole and benzoxadiazole rings. The centroid of the extended π-system formed by the benzoxadiazole and triazole rings (14 atoms total) was calculated; the centroid–centroid distance was 4.179 Å, interplanar separation was 3.243 Å, and the resulting offset was 2.636 Å.

Related literature

For the synthesis of the title compound and related benzoxadiazole analogs, see: Key & Cairo (2011). For computational studies of the absorption and fluorescence properties of this series of compounds, see: Brown *et al.* (2012). For structures with 1-aryl-substituted 1,2,3-triazole rings, see: Costa *et al.* (2006). For the use of fluorophores as chemical or biological probes, see: Cairo *et al.* (2010); Lavis & Raines (2008). For related benzoxadiazole structures, see: Key *et al.* (2012*a*,*b*). For triazole-substituted coumarin derivatives, see: Key *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{17}N_5O$
M_r = 271.33
Triclinic, $P\bar{1}$
a = 5.3604 (8) Å
b = 7.8585 (11) Å
c = 16.357 (2) Å
α = 87.4656 (17)°
β = 86.2519 (16)°
γ = 85.6240 (17)°
V = 685.04 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 K
1.02 × 0.35 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.915, T_{max} = 0.997
6114 measured reflections
3120 independent reflections
2568 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.04
3120 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N2^{i}	0.95	2.52	3.4674 (15)	177
C5—H5···N4^{ii}	0.95	2.46	3.3445 (15)	154

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXD* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2081).

References

Brown, A., Ngai, T. Y., Key, J. A. & Cairo, C. W. (2012). *J. Phys. Chem. A*, **116**, 46–54.
Bruker (2008). *APEX2*, *SAINT* and *SADABS* . Bruker AXS Inc., Madison, Wisconsin, USA.
Cairo, C. W., Key, J. A. & Sadek, C. M. (2010). *Curr. Opin. Chem. Biol.* **14**, 57–63.

Costa, M. S., Boechat, N., Ferreira, V. F., Wardell, S. M. S. V. & Skakle, J. M. S. (2006). *Acta Cryst.* E**62**, o2048–o2050.
Key, J. A. & Cairo, C. W. (2011). *Dyes Pigm.* **88**, 95–102.
Key, J. A., Cairo, C. W. & McDonald, R. (2012*a*). *Acta Cryst.* E**68**, o3130–o3131.
Key, J. A., Cairo, C. W. & McDonald, R. (2012*b*). *Acta Cryst.* E**68**, o3132.
Key, J. A., Koh, S., Timerghazin, Q. K., Brown, A. & Cairo, C. W. (2009). *Dyes Pigm.* **82**, 196–203.
Lavis, L. D. & Raines, R. T. (2008). *ACS Chem. Biol.* **3**, 142–155.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.