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3-(4-Bromophenyl)-2-(3,4-dihydro-2*H*-pyran-5-yl)-1,1,1-trifluoropropan-2-ol

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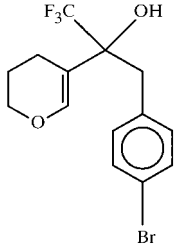
The molecular structure of the title compound, $C_{14}H_{14}BrF_3O_2$, adopts a bent conformation. Intramolecular O—H···F and intermolecular O—H···O interactions form a bifurcated hydrogen bond which produces a supramolecular assembly of head-to-tail dimers.

Comment

The title compound, (I), is an intermediate in the synthesis of trifluoromethyl-substituted naphthalenes (Mellor *et al.*, 2000). Atom C8 forms the central part of a bent structure. The remainder of the molecule adopts the expected geometry, with the ring composed of atoms C10–C14/O2 adopting a six-membered envelope conformation. A strong and highly bent intramolecular interaction occurs; O1—H1···F3 2.785 (4) Å and 104°. In addition, the O1 atom is the donor for a second interaction, creating a bifurcated hydrogen bond. A supramolecular assembly of head-to-tail dimers is formed with O2 as an acceptor; O1—H1···O2 2.921 (5) Å and 166°.



(I)

Experimental

The title compound was prepared *via* a 1,2-addition of *p*-bromobenzyl Grignard to 1-(3,4-dihydro-2*H*-pyran-5-yl)-2,2,2-trifluoro-1-ethanone (Mellor *et al.*, 2000).

Crystal data

$C_{14}H_{14}BrF_3O_2$	$Z = 2$
$M_r = 351.16$	$D_x = 1.627$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.9539$ (16) Å	Cell parameters from 5354 reflections
$b = 9.5523$ (19) Å	$\theta = 2.69$–$27.47°$
$c = 10.695$ (2) Å	$\mu = 2.899$ mm^{-1}
$\alpha = 97.61$ (3)°	$T = 298$ (2) K
$\beta = 110.44$ (3)°	Block, colourless
$\gamma = 104.17$ (3)°	0.35 × 0.35 × 0.35 mm
$V = 716.7$ (2) Å^3	

Data collection

Nonius KappaCCD area-detector diffractometer	2944 independent reflections
φ and ω scans to fill Ewald sphere	1389 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scans (Blessing, 1995)	$R_{int} = 0.0494$
$T_{min} = 0.331$, $T_{max} = 0.379$	$\theta_{max} = 26.00°$
5354 measured reflections	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2 + 0.1443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R(F) = 0.058$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.180$	$\Delta\rho_{max} = 0.44$ e Å^{-3}
$S = 1.002$	$\Delta\rho_{min} = -0.55$ e Å^{-3}
2944 reflections	Extinction correction: *SHELXL*97
182 parameters	Extinction coefficient: 0.015 (4)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Br1—C1	1.887 (6)	C10—C11	1.319 (6)
O1—C8	1.420 (5)	C10—C14	1.497 (6)
O2—C11	1.370 (5)	C12—C13	1.496 (7)
O2—C12	1.435 (6)	C13—C14	1.517 (6)
C4—C7	1.489 (7)		
O1—C8—C7	106.6 (4)	O1—C8—C9	106.0 (3)
O1—C8—C10	112.5 (3)	C7—C8—C9	108.8 (4)
C7—C8—C10	112.8 (3)	C10—C8—C9	109.9 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···F3	0.82	2.47	2.785 (4)	104
O1—H1···O2^{i}	0.82	2.12	2.921 (5)	166

Symmetry code: (i) $2 - x, 3 - y, 2 - z$.

Cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997).

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Mellor, J. M., El-Sagheer, A. H. & Salem, E. E. M. (2000). *Tetrahedron Lett.* Accepted.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.