

Search Overview

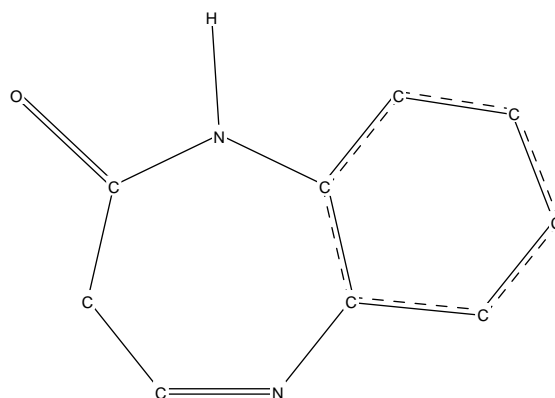
Search: search3
Date/Time done: Wed Nov 28 19:16:15 2018
Database(s): CSD version 5.39 updates (Nov 2017)
CSD version 5.39 (November 2017)
CSD version 5.39 (November 2017)
CSD version 5.39 updates (Feb 2018)
CSD version 5.39 updates (May 2018)
CSD version 5.39 updates (Aug 2018)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 12

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search3 (Wed Nov 28 19:16:15 2018): Hits 1-4

EFARUA

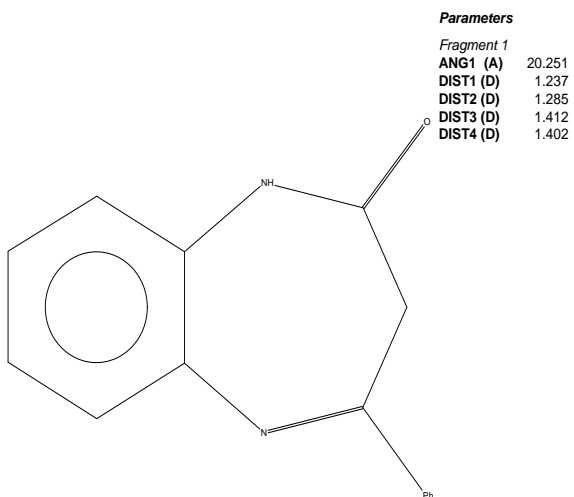
Reference: M.Akkurt, A.R.Kennedy, S.H.H.Younes, S.K.Mohamed, A.A.Abdelhamid (2012) *Acta Crystallogr., Sect.E: Struct.Rep. Online*, **68**, o3356

Formula: C₁₅H₁₂N₂O₁

Compound Name: 4-Phenyl-1H-1,5-benzodiazepin-2(3H)-one

Space Group: P-1 **Cell:** a 4.689(0) b 10.835(1) c 11.754(1)
Space Group No.: 2 **(Å, °)** α 77.72(1) β 83.81(0) γ 82.11(1)

R-Factor (%): 5.34 **Temperature(K):** 123 **Density(g/cm³):** 1.362



INIZUC

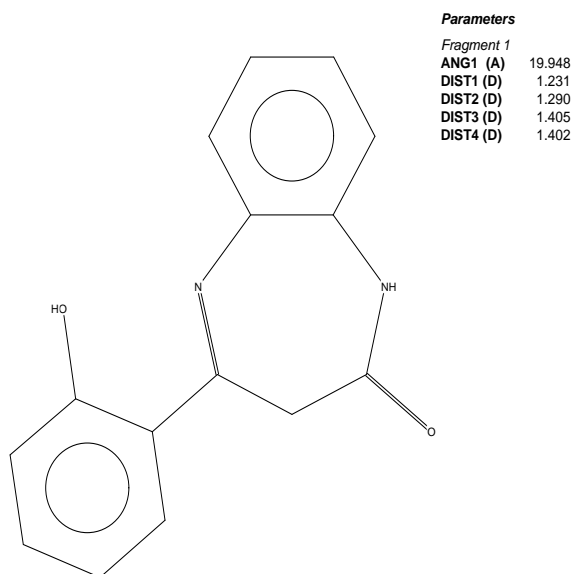
Reference: H.Miraoui, R.Gharbi, M.Msaddek, Y.Bretonniere, C.Andraud, C.Sabot, P.-Y.Renard (2016) *J.Org.Chem.*, **81**,4720

Formula: C₁₅H₁₂N₂O₂

Compound Name: 4-(2-hydroxyphenyl)-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P21/n **Cell:** a 4.692(0) b 12.148(2) c 21.030(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.01(0) γ 90.00

R-Factor (%): 4.20 **Temperature(K):** 293 **Density(g/cm³):** 1.403



JARBOW

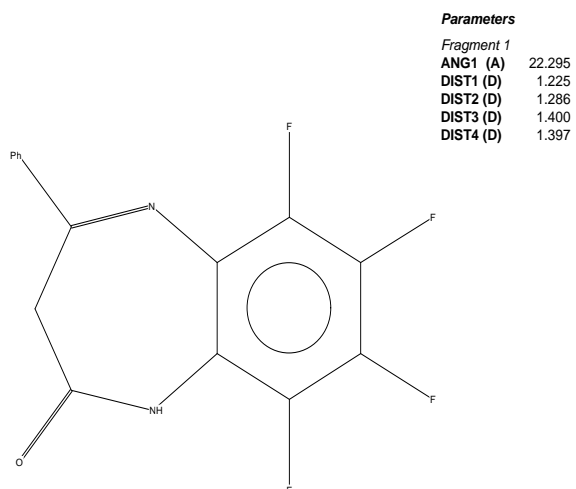
Reference: O.Martin, M.Perez-Torraiba, M.Angeles Garcia, R.M.Claramunt, M.Carmen Torralba, M.Rosario Torres, I.Alkorta, J.Elguero (2016) *Chem. Sel.*, **1**,861

Formula: C₁₅H₈F₄N₂O₁

Compound Name: 6,7,8,9-tetrafluoro-4-phenyl-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P21/c **Cell:** a 13.035(3) b 6.981(1) c 15.450(4)
Space Group No.: 14 **(Å, °)** α 90.00 β 110.70(0) γ 90.00

R-Factor (%): 4.34 **Temperature(K):** 296 **Density(g/cm³):** 1.557



JARBUC

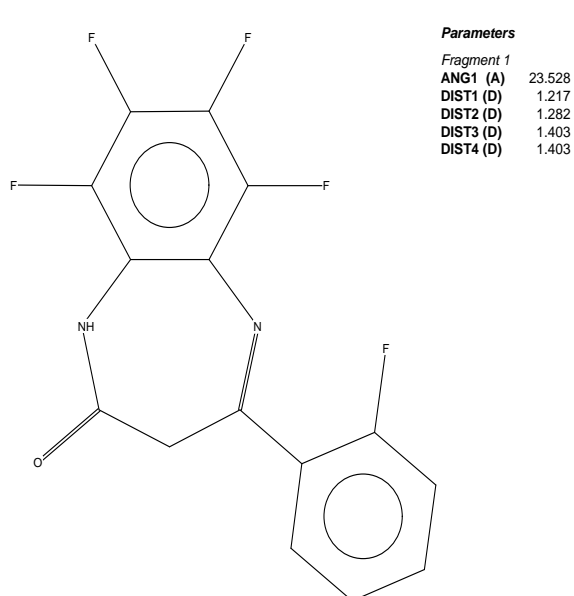
Reference: O.Martin, M.Perez-Torraiba, M.Angeles Garcia, R.M.Claramunt, M.Carmen Torralba, M.Rosario Torres, I.Alkorta, J.Elguero (2016) *Chem. Sel.*, **1**,861

Formula: C₁₅H₇F₅N₂O₁

Compound Name: 6,7,8,9-tetrafluoro-4-(2-fluorophenyl)-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P21/n **Cell:** a 6.502 b 25.870 c 7.913
Space Group No.: 14 **(Å, °)** α 90.00 β 106.87 γ 90.00

R-Factor (%): 4.07 **Temperature(K):** 293 **Density(g/cm³):** 1.701



Search: search3 (Wed Nov 28 19:16:15 2018): Hits 5-8

JARCAJ

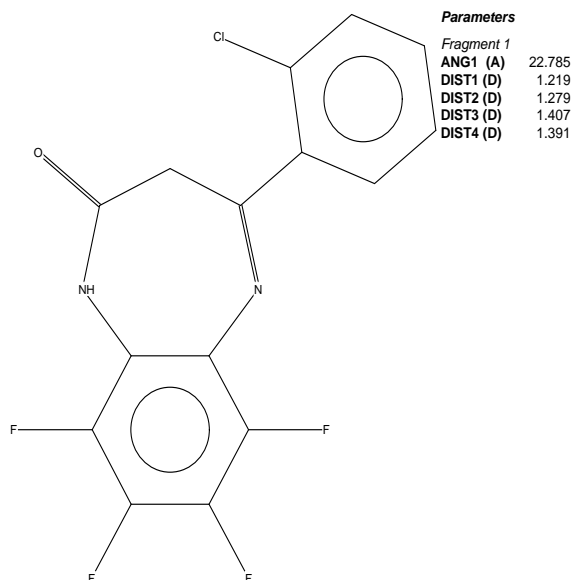
Reference: O.Martin, M.Perez-Torralba, M.Angeles Garcia, R.M.Claramunt, M.Carmen Torralba, M.Rosario Torres, I.Alkorta, J.Elguero (2016) *Chem. Sel.*, 1,861

Formula: C₁₅ H₇ Cl₁ F₄ N₂ O₁

Compound Name: 4-(2-chlorophenyl)-6,7,8,9-tetrafluoro-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P-1 **Cell:** a 7.654(2) b 7.845(2) c 12.462(3)
Space Group No.: 2 **(Å, °)** α 93.29(0) β 106.39(0) γ 108.61(0)

R-Factor (%): 4.42 **Temperature(K):** 296 **Density(g/cm³):** 1.695



MOMBAT

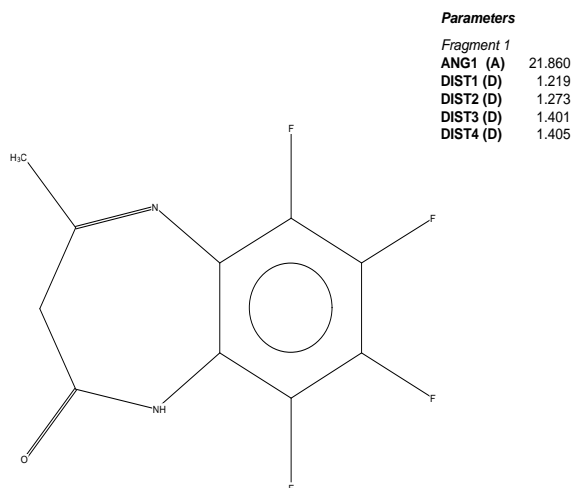
Reference: M.Perez-Torralba, R.M.Claramunt, M.Angeles Garcia, C.Lopez, M.Carmen Torralba, M.Rosario Torres, I.Alkorta, J.Elguero (2013) *Beilstein J.Org.Chem.*, 9,2156

Formula: C₁₀ H₆ F₄ N₂ O₁

Compound Name: 6,7,8,9-Tetrafluoro-4-methyl-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P21/c **Cell:** a 5.282(0) b 18.255(1) c 10.210(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.93(1) γ 90.00

R-Factor (%): 3.86 **Temperature(K):** 293 **Density(g/cm³):** 1.691



TALSEH

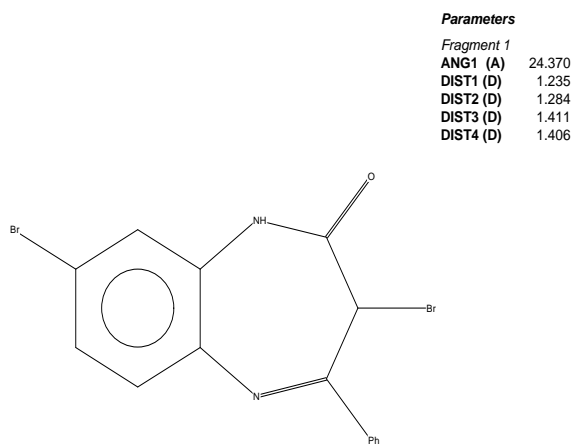
Reference: A.Essaghouni, M.Boulhaoua, S.Lahmidi, M.M.Mohamed Abdelahi, E.M.Essassi, J.T.Mague (2017) *IUCrData*, 2, x170389

Formula: C₁₅ H₁₀ Br₂ N₂ O₁

Compound Name: (3S)-3,8-dibromo-4-phenyl-2,3-dihydro-1H-1,5-benzodiazepine-2-one

Space Group: P-1 **Cell:** a 7.893(0) b 9.930(1) c 10.241(1)
Space Group No.: 2 **(Å, °)** α 101.75(0) β 105.97(0) γ 109.48(0)

R-Factor (%): 2.82 **Temperature(K):** 100 **Density(g/cm³):** 1.903



TUPSAZ

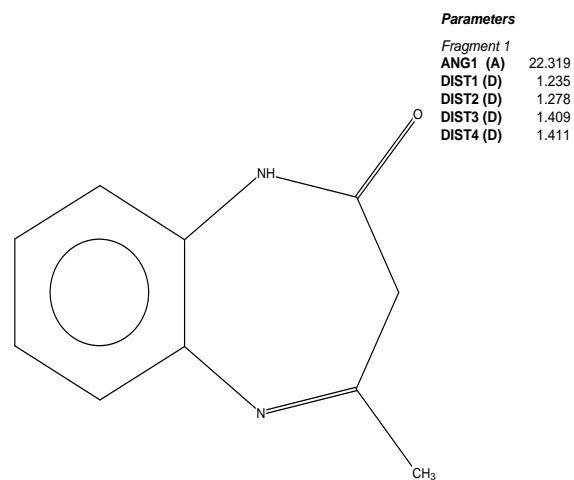
Reference: A.Saber, H.Zouihri, E.M.Essassi, S.W.Ng (2010) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, 66, o1408

Formula: C₁₀ H₁₀ N₂ O₁·H₂ O₁

Compound Name: 4-Methyl-2,3-dihydro-1H-1,5-benzodiazepin-2-one monohydrate

Space Group: P-1 **Cell:** a 4.901(0) b 7.315(0) c 13.569(0)
Space Group No.: 2 **(Å, °)** α 85.38(0) β 83.96(0) γ 83.81(0)

R-Factor (%): 3.81 **Temperature(K):** 100 **Density(g/cm³):** 1.331



Search: search3 (Wed Nov 28 19:16:15 2018): Hits 9-12

XOTQAA

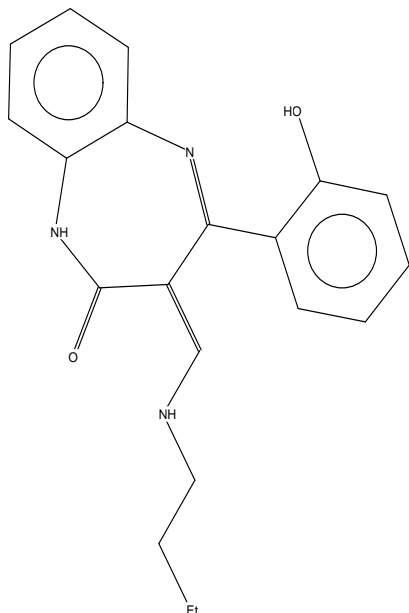
Reference: S.CHNITI (2014)
CSD Communication(Private Communication),

Formula: C₂₀H₂₁N₃O₂

Compound Name: 3-((butylamino)methylene)-4-(2-hydroxyphenyl)-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: C2/c **Cell:** a 26.091(1) b 9.078(0) c 15.143(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 97.26(0) γ 90.00

R-Factor (%): 6.32 **Temperature(K):** 293 **Density(g/cm³):** 1.252



Parameters

Fragment 1	
ANG1 (A)	22.278
DIST1 (D)	1.241
DIST2 (D)	1.295
DIST3 (D)	1.412
DIST4 (D)	1.400

ZISQOJ

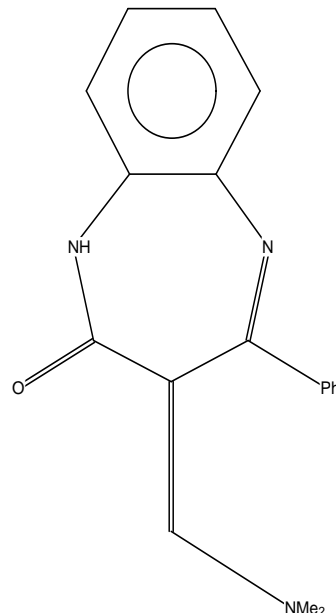
Reference: M.Loughzail, A.Baouid, J.A.Fernandes, M.Driss, E.H.Soumhi (2014) Acta Crystallogr., Sect. E: Struct. Rep. Online, 70, o126

Formula: C₁₈H₁₇N₃O₁

Compound Name: (E)-3-((Dimethylamino)methylene)-4-phenyl-1,3-dihydro-2H-1,5-benzodiazepin-2-one

Space Group: P21/n **Cell:** a 11.281(2) b 14.005(4) c 20.124(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.97(1) γ 90.00

R-Factor (%): 5.15 **Temperature(K):** 300 **Density(g/cm³):** 1.224



Parameters

Fragment 1	
ANG1 (A)	25.170
DIST1 (D)	1.234
DIST2 (D)	1.285
DIST3 (D)	1.404
DIST4 (D)	1.405

Parameters

Fragment 2	
ANG1 (A)	29.161
DIST1 (D)	1.229
DIST2 (D)	1.285
DIST3 (D)	1.410
DIST4 (D)	1.404

ZUFQAU

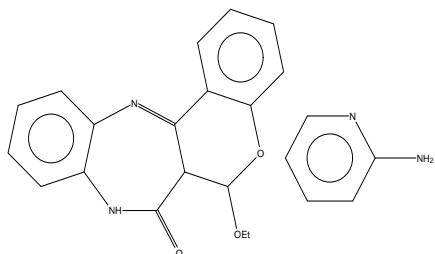
Reference: A.Nsira, R.Gharbi, M.Msaddek (2014)
Comptes Rendus Chimie, 17,1242

Formula: C₁₈H₁₆N₂O₃.C₅H₆N₂

Compound Name: 6-ethoxy-6a,8-dihydrochromeno[4,3-b][1,5]benzodiazepin-7(6H)-one pyridin-2-amine

Space Group: P-1 **Cell:** a 6.849(5) b 10.387(5) c 15.298(5)
Space Group No.: 2 **(Å, °)** α 106.25(0) β 91.10(0) γ 97.94(0)

R-Factor (%): 4.20 **Temperature(K):** 150 **Density(g/cm³):** 1.294



Parameters

Fragment 1	
ANG1 (A)	25.488
DIST1 (D)	1.232
DIST2 (D)	1.282
DIST3 (D)	1.415
DIST4 (D)	1.414

GESFOC

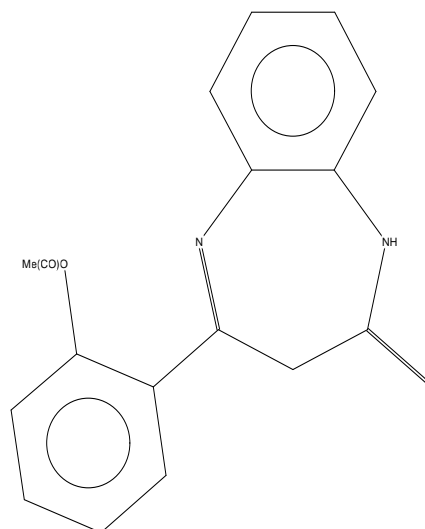
Reference: H.Miraoui, A.Nsira, M.Msaddek, P.-Y.Renard, C.Sabot (2017) Comptes Rendus Chimie, 20,747

Formula: C₁₇H₁₄N₂O₃

Compound Name: 2-(2-oxo-2,3-dihydro-1H-1,5-benzodiazepin-4-yl)phenyl acetate

Space Group: P21/c **Cell:** a 6.240(1) b 13.015(2) c 17.705(3)
Space Group No.: 14 **(Å, °)** α 90.00 β 97.00(0) γ 90.00

R-Factor (%): 5.49 **Temperature(K):** 293 **Density(g/cm³):** 1.370



Parameters

Fragment 1	
ANG1 (A)	25.022
DIST1 (D)	1.235
DIST2 (D)	1.278
DIST3 (D)	1.415
DIST4 (D)	1.406