

Search Overview

Search: search2
Date/Time done: Sun Oct 13 16:31:09 2019
Database(s): CSD version 5.40 updates (Feb 2019)
CSD version 5.40 (November 2018)
CSD version 5.40 updates (May 2019)
CSD version 5.40 updates (Aug 2019)
Restriction Info: No refcode restrictions applied
Filters: None
Percentage Completed: 100%
Number of Hits: 7

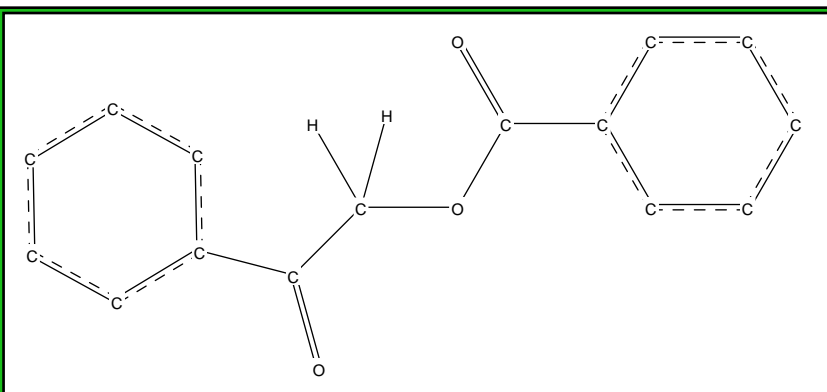
Summary of queries used. Search found structures that:

match

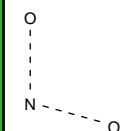
Query 1

Query 2

Query 1



Query 2



Search: search2 (Sun Oct 13 16:31:09 2019): Hits 1-4

CISRUU

Reference: Huey Chong Kwong, C.S.Chidan Kumar, Siau Hui Mah, Tze Shyang Chia, Ching Kheng Quah, Zi Han Loh, S.Chandrajou, Gin Keat Lim (2017) *Plos One* ,12,e0170117

Formula: C₂₁ H₁₅ N₁ O₅

Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-nitrobenzoate

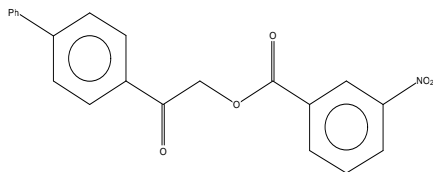
Space Group: P-1 **Cell:** a 4.933(0) b 18.312(1) c 19.167(1)
Space Group No.: 2 **(Å, °)** α 103.22(0) β 97.41(0) γ 89.98(0)

R-Factor (%): 4.21 **Temperature(K):** 100 **Density(g/cm³):** 1.437

Parameters

Fragment 1
ANG1 (A) 64.060
ANG2 (A) 69.594
ANG3 (A) 65.756

Fragment 2
ANG1 (A) 64.087
ANG2 (A) 69.652
ANG3 (A) 65.704



CISSAB

Reference: Huey Chong Kwong, C.S.Chidan Kumar, Siau Hui Mah, Tze Shyang Chia, Ching Kheng Quah, Zi Han Loh, S.Chandrajou, Gin Keat Lim (2017) *Plos One* ,12,e0170117

Formula: C₂₁ H₁₅ N₁ O₅

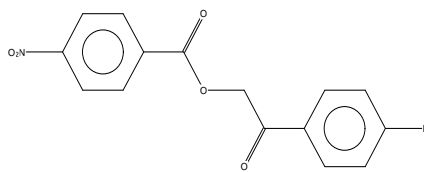
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 4-nitrobenzoate

Space Group: P21/c **Cell:** a 8.681(1) b 5.555(0) c 35.401(5)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.12(0) γ 90.00

R-Factor (%): 5.26 **Temperature(K):** 293 **Density(g/cm³):** 1.406

Parameters

Fragment 1
ANG1 (A) 70.959
ANG2 (A) 42.607
ANG3 (A) 82.524



JIVJOQ

Reference: Huey Chong Kwong, C.S.Chidan Kumar, Siau Hui Mah, Tze Shyang Chia, Ching Kheng Quah, Zi Han Loh, S.Chandrajou, Gin Keat Lim (2017) *Plos One* ,12,e0170117

Formula: C₂₁ H₁₅ N₁ O₅

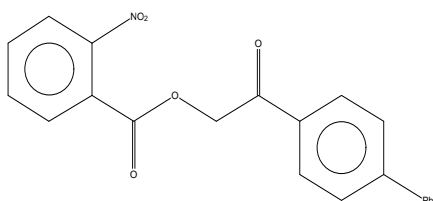
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2-nitrobenzoate

Space Group: Pna21 **Cell:** a 9.844(1) b 32.312(5) c 5.368(0)
Space Group No.: 33 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.54 **Temperature(K):** 100 **Density(g/cm³):** 1.406

Parameters

Fragment 1
ANG1 (A) 11.771
ANG2 (A) 58.652
ANG3 (A) 61.685



CIYCAQ

Reference: C.S.C.Kumar, Tze Shyang Chia, S.Chandrajou, Chin Wei Ooi, Ching Kheng Quah, Hoong-Kun Fun (2014) *Z.Krist.Cryst.Mater.* ,229,328

Formula: C₁₅ H₁₀ Br₁ N₁ O₅

Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 2-nitrobenzoate

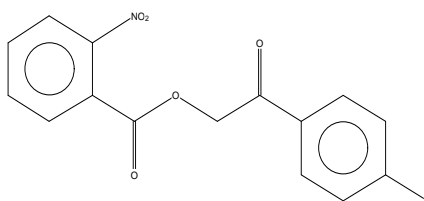
Space Group: P21/c **Cell:** a 15.596(1) b 25.103(3) c 7.254(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 99.44(0) γ 90.00

R-Factor (%): 3.83 **Temperature(K):** 100 **Density(g/cm³):** 1.727

Parameters

Fragment 1
ANG1 (A) 24.998
ANG2 (A) 57.508
ANG3 (A) 65.709

Fragment 2
ANG1 (A) 69.517
ANG2 (A) 40.068
ANG3 (A) 89.505



Search: search2 (Sun Oct 13 16:31:09 2019): Hits 5-7

CIYCEU

Reference: C.S.C.Kumar, Tze Shyang Chia, S.Chandrajua,
Chin Wei Ooi, Ching Kheng Quah, Hoong-Kun Fun (2014)
Z.Krist.Cryst.Mater. ,229,328

Formula: C₁₅ H₁₀ Br₁ N₁ O₅

Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 3-nitrobenzoate

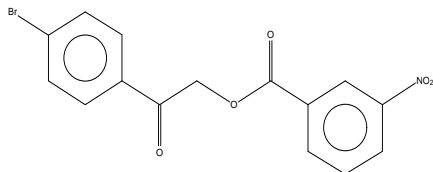
Space Group: P-1 **Cell:** a 9.311(0) b 12.098(1) c 14.175(1)
Space Group No.: 2 **(Å, °)** α 100.61(0) β 100.35(0) γ 105.99(0)

R-Factor (%): 5.48 **Temperature(K):** 296 **Density(g/cm³):** 1.653

Parameters

Fragment 1
ANG1 (A) 4.742
ANG2 (A) 1.620
ANG3 (A) 4.446

Fragment 2
ANG1 (A) 7.368
ANG2 (A) 3.781
ANG3 (A) 4.080



CIYCIY

Reference: C.S.C.Kumar, Tze Shyang Chia, S.Chandrajua,
Chin Wei Ooi, Ching Kheng Quah, Hoong-Kun Fun (2014)
Z.Krist.Cryst.Mater. ,229,328

Formula: C₁₅ H₁₀ Br₁ N₁ O₅

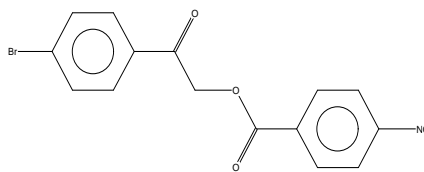
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-nitrobenzoate

Space Group: P21/c **Cell:** a 14.896(0) b 12.707(0) c 7.371(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 96.20(0) γ 90.00

R-Factor (%): 4.45 **Temperature(K):** 100 **Density(g/cm³):** 1.744

Parameters

Fragment 1
ANG1 (A) 82.031
ANG2 (A) 38.088
ANG3 (A) 87.661



PODRAD

Reference: C.S.Chidan Kumar, C.Yohannan Panicker,
Hoong-Kun Fun, Y.Sheena Mary, B.Harikumar, S.Chandrajua,
Ching Kheng Quah, Chin Wei Ooi (2014) *Spectrochim.Acta,Part A* ,
126,208

Formula: C₁₅ H₁₀ Cl₁ N₁ O₅

Compound Name: 2-(4-chlorophenyl)-2-oxoethyl 3-nitrobenzoate

Space Group: P-1 **Cell:** a 9.258(1) b 12.106(1) c 14.123(1)
Space Group No.: 2 **(Å, °)** α 100.79(0) β 100.20(1) γ 106.21(0)

R-Factor (%): 5.60 **Temperature(K):** 297 **Density(g/cm³):** 1.466

Parameters

Fragment 1
ANG1 (A) 3.702
ANG2 (A) 2.438
ANG3 (A) 3.207

Fragment 2
ANG1 (A) 5.918
ANG2 (A) 3.974
ANG3 (A) 2.999

