

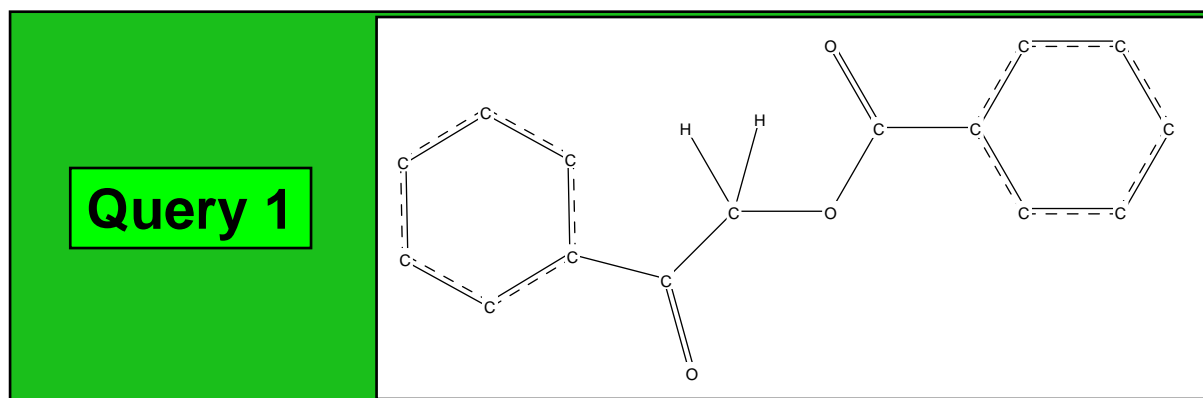
Search Overview

Search: search1
Date/Time done: Sun Oct 13 16:24:06 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: 62

Single query used. Search found structures that:

match

Query 1



Search: search1 (Sun Oct 13 16:24:06 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: C₂₁H₁₅N₁O₅

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

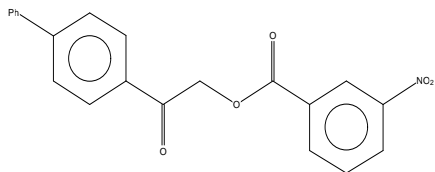
Space Group: P-1 **Cell:** a 4.933(0) b 18.312(1) c 19.167(1)
Space Group No.: 2 **(Å, °)** α 103.22(0) β 97.41(0) γ 89.98(0)

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

Parameters

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

Fragment 2
ANG1 (Å) 64.087
ANG2 (Å) 69.652
ANG3 (Å) 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: C₂₁H₁₅N₁O₅

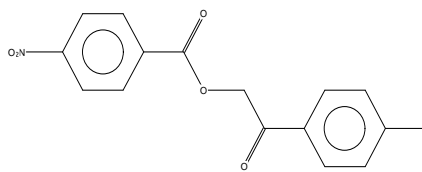
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 4-nitrobenzoate

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 (Å) 70.959
ANG2 (Å) 42.607
ANG3 (Å) 82.524



CISSEF

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: C₂₁H₁₇N₁O₃

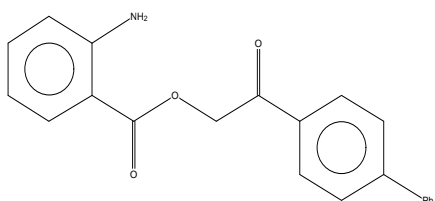
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2-aminobenzoate

Space Group: Pbc_a **Cell:** a 10.661(1) b 9.824(1) c 32.235(4)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.82 **Temperature(K):** 294 **Density(g/cm³):** 1.304

Parameters

Fragment 1
ANG1 (Å) 52.331
ANG2 (Å) 52.868
ANG3 (Å) 55.822



CISSIJ

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: C₂₁H₁₇N₁O₃

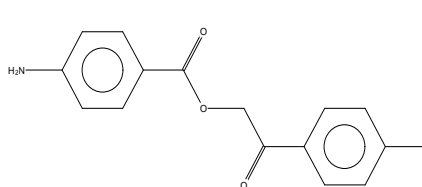
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 4-aminobenzoate

Space Group: P21 **Cell:** a 8.330(0) b 5.065(0) c 19.467(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 95.71(0) γ 90.00

R-Factor (%): 3.63 **Temperature(K):** 100 **Density(g/cm³):** 1.347

Parameters

Fragment 1
ANG1 (Å) 78.446
ANG2 (Å) 70.856
ANG3 (Å) 65.332



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 5-8

GESBUE01

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 H₁₇ N₁ O₃

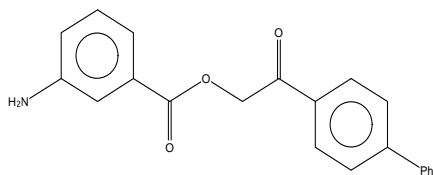
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-aminobenzoate

Space Group: P-1 **Cell:** a 5.293(0) b 11.682(1) c 13.404(1)
Space Group No.: 2 **(Å,°)** α 87.86(0) β 83.98(0) γ 87.70(0)

R-Factor (%): 5.45 **Temperature(K):** 294 **Density(g/cm³):** 1.337

Parameters

Fragment 1
ANG1 (Å) 75.690
ANG2 (Å) 45.492
ANG3 (Å) 61.521



JIVHAA

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 Cl₁ O₃

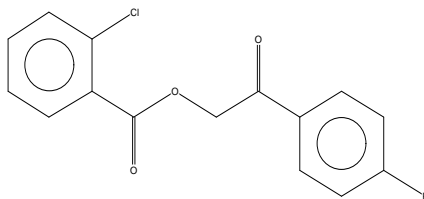
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2-chlorobenzoate

Space Group: Pbca **Cell:** a 11.397(1) b 8.036(1) c 36.509(6)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.50 **Temperature(K):** 100 **Density(g/cm³):** 1.394

Parameters

Fragment 1
ANG1 (Å) 74.357
ANG2 (Å) 86.176
ANG3 (Å) 52.373



JIVHEE

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: C₂₂ H₁₈ O₃

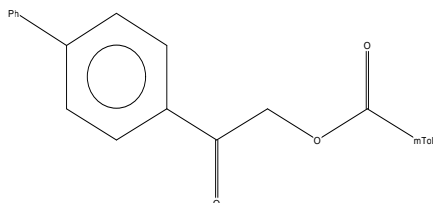
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-methylbenzoate

Space Group: P21 **Cell:** a 5.288(1) b 8.975(2) c 17.996(4)
Space Group No.: 4 **(Å,°)** α 90.00 β 93.83(0) γ 90.00

R-Factor (%): 4.60 **Temperature(K):** 294 **Density(g/cm³):** 1.288

Parameters

Fragment 1
ANG1 (Å) 77.591
ANG2 (Å) 61.341
ANG3 (Å) 54.645



JIVHII

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 Cl₁ O₃

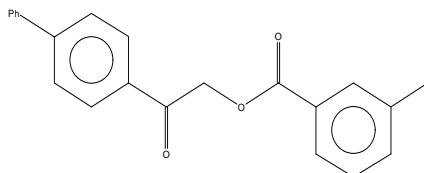
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-chlorobenzoate

Space Group: P21/c **Cell:** a 5.026(0) b 9.277(1) c 36.530(4)
Space Group No.: 14 **(Å,°)** α 90.00 β 91.23(0) γ 90.00

R-Factor (%): 4.76 **Temperature(K):** 294 **Density(g/cm³):** 1.368

Parameters

Fragment 1
ANG1 (Å) 56.619
ANG2 (Å) 81.410
ANG3 (Å) 64.521



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 9-12

JIVHOO

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: C₂₁H₁₄Cl₂O₃

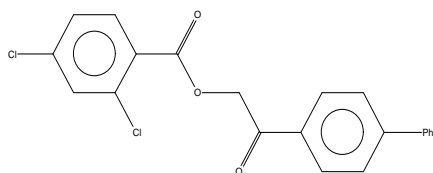
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2,4-dichlorobenzoate

Space Group: P21/c **Cell:** a 12.543(1) b 8.658(0) c 17.446(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 108.99(0) γ 90.00

R-Factor (%): 5.06 **Temperature(K):** 294 **Density(g/cm³):** 1.428

Parameters

Fragment 1
ANG1 (A) 77.636
ANG2 (A) 53.831
ANG3 (A) 65.242



JIVHUU

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: C₂₂H₁₈O₄

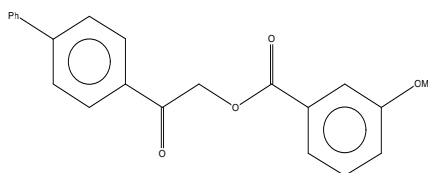
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-methoxybenzoate

Space Group: P21/c **Cell:** a 10.725(0) b 9.072(0) c 17.368(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 93.34(0) γ 90.00

R-Factor (%): 4.23 **Temperature(K):** 100 **Density(g/cm³):** 1.364

Parameters

Fragment 1
ANG1 (A) 76.009
ANG2 (A) 56.765
ANG3 (A) 68.811



JIVJAC

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: C₂₁H₁₅Cl₁O₃

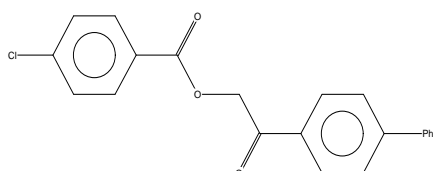
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 4-chlorobenzoate

Space Group: Pbc_a **Cell:** a 9.715(0) b 9.439(0) c 36.285(2)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.91 **Temperature(K):** 100 **Density(g/cm³):** 1.401

Parameters

Fragment 1
ANG1 (A) 43.718
ANG2 (A) 56.942
ANG3 (A) 51.884



JIVJEG

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: C₂₂H₁₈O₄

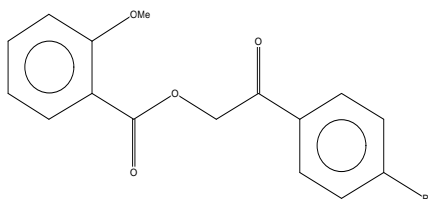
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2-methoxybenzoate

Space Group: Pbc_a **Cell:** a 17.341(2) b 8.920(1) c 22.412(3)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.16 **Temperature(K):** 100 **Density(g/cm³):** 1.327

Parameters

Fragment 1
ANG1 (A) 62.833
ANG2 (A) 55.977
ANG3 (A) 80.097



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 13-16

JIVJIK

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: C₂₂H₁₈O₄

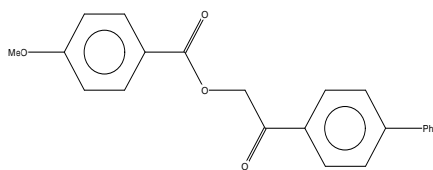
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 4-methoxybenzoate

Space Group: P21 **Cell:** a 8.659(1) b 5.269(0) c 19.270(3)
Space Group No.: 4 **(Å,°)** α 90.00 β 91.78(0) γ 90.00

R-Factor (%): 4.43 **Temperature(K):** 294 **Density(g/cm³):** 1.309

Parameters

Fragment 1
ANG1 (Å) 75.291
ANG2 (Å) 58.878
ANG3 (Å) 54.645



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: C₂₁H₁₅N₁O₅

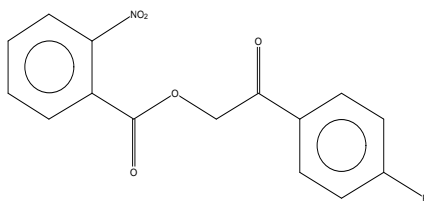
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 2-nitrobenzoate

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 (Å) 11.771
ANG2 (Å) 58.652
ANG3 (Å) 61.685



AZULUD

Reference: H.-K.Fun, T.Shahani, B.Garudachari, A.M.Isloor, K.N.Shivananda (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,67, o2682

Formula: C₁₅H₁₁Cl₁O₄

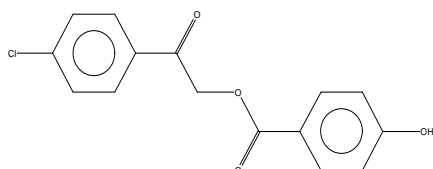
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 4-hydroxybenzoate

Space Group: P21 **Cell:** a 5.531(1) b 8.132(1) c 14.857(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 95.12(0) γ 90.00

R-Factor (%): 4.43 **Temperature(K):** 296 **Density(g/cm³):** 1.451

Parameters

Fragment 1
ANG1 (Å) 65.702
ANG2 (Å) 51.592
ANG3 (Å) 53.658



BOQXOW

Reference: I.Khan, A.Ibrar, S.Hameed, J.M.White, J.Simpson (2014) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,70,301

Formula: C₁₅H₁₀Br₁Cl₁O₃

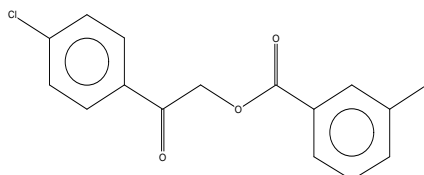
Compound Name: 2-(4-chlorophenyl)-2-oxoethyl 3-bromobenzoate

Space Group: P-1 **Cell:** a 6.680(0) b 10.024(0) c 10.785(0)
Space Group No.: 2 **(Å,°)** α 90.98(0) β 107.57(0) γ 92.14(0)

R-Factor (%): 2.66 **Temperature(K):** 130 **Density(g/cm³):** 1.708

Parameters

Fragment 1
ANG1 (Å) 86.110
ANG2 (Å) 50.650
ANG3 (Å) 79.121



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 17-20

CIQNEW

Reference: Tao Ji, Xi-Lin Wang, Yu-Xing Gao, Guo Tang, Yu-Fen Zhao (2007) *Acta Crystallogr., Sect. E: Struct. Rep. Online*, **63**, o4766

Formula: C₁₆H₁₄O₄

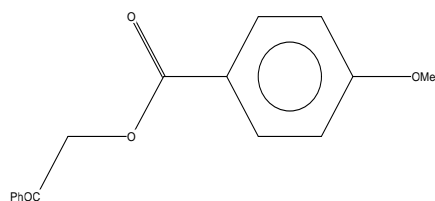
Compound Name: Benzoylmethyl 4-methoxybenzoate

Space Group: P2₁/n **Cell:** a 8.062(0) b 9.667(0) c 17.182(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 91.53(0) γ 90.00

R-Factor (%): 3.46 **Temperature(K):** 298 **Density(g/cm³):** 1.341

Parameters

Fragment 1
ANG1 (Å) 71.209
ANG2 (Å) 59.553
ANG3 (Å) 53.755



CIXVUC

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: C₁₅H₁₀Br₁Cl₁O₃

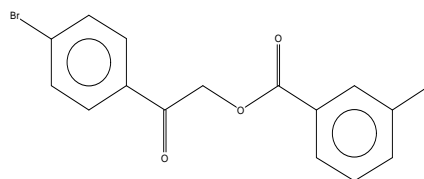
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 3-chlorobenzoate

Space Group: P-1 **Cell:** a 6.722(0) b 10.194(1) c 10.889(1)
Space Group No.: 2 **(Å, °)** α 91.67(0) β 107.64(0) γ 90.91(0)

R-Factor (%): 2.64 **Temperature(K):** 296 **Density(g/cm³):** 1.653

Parameters

Fragment 1
ANG1 (Å) 85.170
ANG2 (Å) 51.606
ANG3 (Å) 77.905



CIXWAJ

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: C₁₅H₉Br₁Cl₂O₃

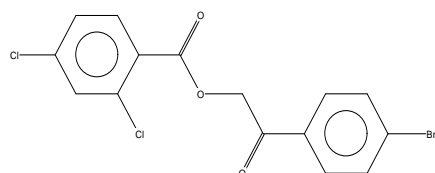
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 2,4-dichlorobenzoate

Space Group: C2/c **Cell:** a 28.309(2) b 12.132(0) c 8.798(0)
Space Group No.: 15 **(Å, °)** α 90.00 β 97.71(0) γ 90.00

R-Factor (%): 4.45 **Temperature(K):** 296 **Density(g/cm³):** 1.721

Parameters

Fragment 1
ANG1 (Å) 6.166
ANG2 (Å) 6.156
ANG3 (Å) 0.062



CIXWEN

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: C₁₅H₁₂Br₁N₁O₃

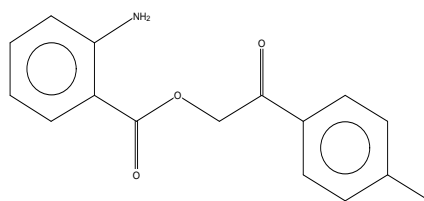
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 2-aminobenzoate

Space Group: P2₁/c **Cell:** a 15.295(2) b 9.870(1) c 9.413(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 93.62(0) γ 90.00

R-Factor (%): 4.87 **Temperature(K):** 296 **Density(g/cm³):** 1.565

Parameters

Fragment 1
ANG1 (Å) 83.028
ANG2 (Å) 70.499
ANG3 (Å) 61.438



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 21-24

CIXWIR

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 H₁₂ Br₁ N₁ O₃

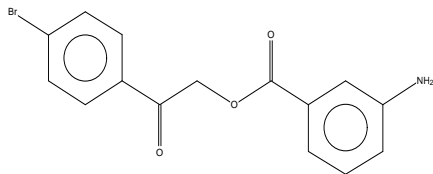
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 3-aminobenzoate

Space Group: P21/c **Cell:** a 8.215(1) b 10.592(1) c 17.117(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 110.95(0) γ 90.00

R-Factor (%): 4.78 **Temperature(K):** 296 **Density(g/cm³):** 1.596

Parameters

Fragment 1
ANG1 (Å) 84.091
ANG2 (Å) 49.757
ANG3 (Å) 73.834



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

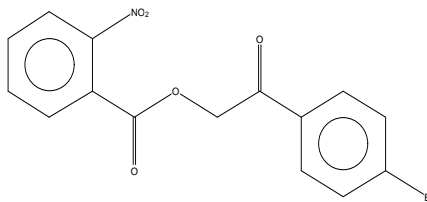
Space Group: P21/c **Cell:** a 15.596(1) b 25.103(3) c 7.254(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 99.44(0) γ 90.00

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

Parameters

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

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



CIYCEU

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 3-nitrobenzoate

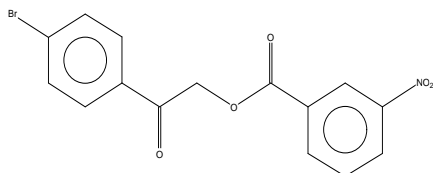
Space Group: P-1 **Cell:** a 9.311(0) b 12.098(1) c 14.175(1)
Space Group No.: 2 **(Å,°)** α 100.61(0) β 100.35(0) γ 105.99(0)

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

Parameters

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

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



CIYCIY

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

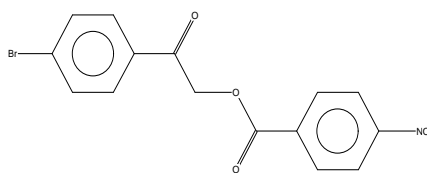
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-nitrobenzoate

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 (Å) 82.031
ANG2 (Å) 38.088
ANG3 (Å) 87.661



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 25-28

CIYCOE

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

Formula: C₁₅H₁₂Br₁N₁O₃

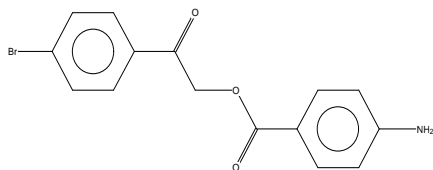
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-aminobenzoate

Space Group: P212121 **Cell:** a 5.250(1) b 8.271(1) c 32.035(6)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.62 **Temperature(K):** 296 **Density(g/cm³):** 1.596

Parameters

Fragment 1
ANG1 (Å) 75.973
ANG2 (Å) 57.749
ANG3 (Å) 53.378



CIYFUN

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

Formula: C₁₅H₁₁Br₁O₃

Compound Name: 2-(4-bromophenyl)-2-oxoethyl benzoate

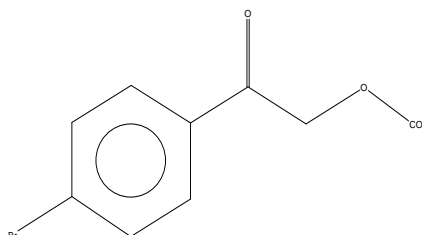
Space Group: P21/c **Cell:** a 8.393(0) b 10.458(1) c 31.286(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 92.53(0) γ 90.00

R-Factor (%): 5.35 **Temperature(K):** 296 **Density(g/cm³):** 1.545

Parameters

Fragment 1
ANG1 (Å) 68.699
ANG2 (Å) 44.352
ANG3 (Å) 53.624

Fragment 2
ANG1 (Å) 72.430
ANG2 (Å) 52.078
ANG3 (Å) 46.758



CIYGAI

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

Formula: C₁₅H₁₀Br₁Cl₁O₃

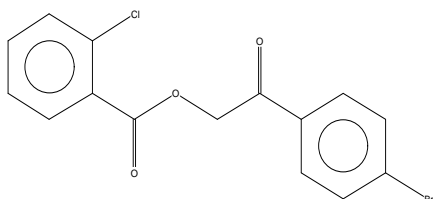
Compound Name: 2-(4-bromophenyl)-2-oxoethyl 2-chlorobenzoate

Space Group: Pbc_a **Cell:** a 12.326(1) b 8.353(0) c 27.305(3)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.79 **Temperature(K):** 296 **Density(g/cm³):** 1.671

Parameters

Fragment 1
ANG1 (Å) 6.555
ANG2 (Å) 5.832
ANG3 (Å) 1.619



EVAFOX

Reference: H.-K.Fun, S.Arshad, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online* **67**,o1582

Formula: C₁₅H₁₀Br₂O₃

Compound Name: 2-(4-bromophenyl)-2-oxoethyl 4-bromobenzoate

Space Group: P_c **Cell:** a 11.048(0) b 5.908(0) c 33.855(0)
Space Group No.: 7 **(Å,°)** α 90.00 β 108.80(0) γ 90.00

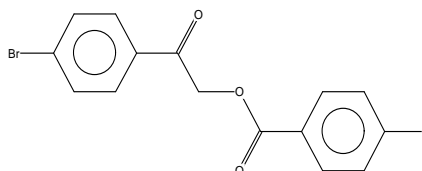
R-Factor (%): 4.73 **Temperature(K):** 100 **Density(g/cm³):** 1.896

Parameters

Fragment 1
ANG1 (Å) 3.157
ANG2 (Å) 3.347
ANG3 (Å) 4.064

Fragment 2
ANG1 (Å) 54.590
ANG2 (Å) 33.377
ANG3 (Å) 53.965

Fragment 3
ANG1 (Å) 6.081
ANG2 (Å) 5.580
ANG3 (Å) 6.130



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 29-32

EVAJAN

Reference: H.-K.Fun, W.-S.Loh, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1597

Formula: C₁₆H₁₀Cl₁F₃O₃

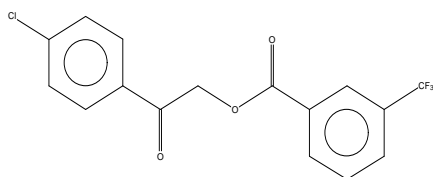
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate

Space Group: P21/c **Cell:** a 14.304(0) b 12.133(0) c 8.546(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 101.44(0) γ 90.00

R-Factor (%): 4.83 **Temperature(K):** 100 **Density(g/cm³):** 1.566

Parameters

Fragment 1
ANG1 (Å) 15.498
ANG2 (Å) 3.575
ANG3 (Å) 14.427



EVAJIV

Reference: H.-K.Fun, S.Arshad, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1599

Formula: C₁₅H₉Cl₁F₂O₃

Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 2,4-difluorobenzoate

Space Group: P21/c **Cell:** a 16.018(1) b 7.961(0) c 24.017(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 115.94(0) γ 90.00

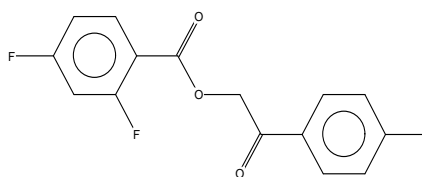
R-Factor (%): 5.42 **Temperature(K):** 296 **Density(g/cm³):** 1.499

Parameters

Fragment 1
ANG1 (Å) 7.922
ANG2 (Å) 19.331
ANG3 (Å) 12.874

Fragment 2

ANG1 (Å) 73.504
ANG2 (Å) 49.205
ANG3 (Å) 60.714



EVAZEH

Reference: H.-K.Fun, S.I.J.Asik, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1687

Formula: C₁₆H₁₃Cl₁O₄

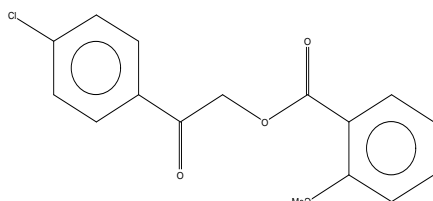
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 2-methoxybenzoate

Space Group: Pbc_a **Cell:** a 7.721(0) b 14.441(1) c 26.064(2)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 296 **Density(g/cm³):** 1.393

Parameters

Fragment 1
ANG1 (Å) 86.378
ANG2 (Å) 47.391
ANG3 (Å) 75.422



EVEGIW

Reference: H.-K.Fun, C.S.Yeap, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1723

Formula: C₁₅H₁₀Br₁Cl₁O₃

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

Space Group: P21 **Cell:** a 17.106(1) b 5.306(0) c 24.038(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 101.50(0) γ 90.00

R-Factor (%): 4.49 **Temperature(K):** 297 **Density(g/cm³):** 1.648

Parameters

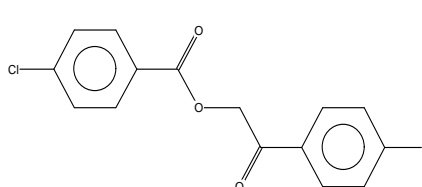
Fragment 1
ANG1 (Å) 0.745
ANG2 (Å) 3.455
ANG3 (Å) 3.889

Fragment 2

ANG1 (Å) 66.087
ANG2 (Å) 49.602
ANG3 (Å) 52.536

Fragment 3

ANG1 (Å) 68.779
ANG2 (Å) 49.032
ANG3 (Å) 54.911



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 33-36

EVEGOC

Reference: H.-K.Fun, C.K.Quah, B.Garudachari, A.M.Isloor, M.N.Satygarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1724

Formula: C₁₆H₁₃Br₁O₄

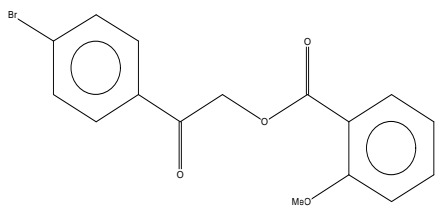
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 2-methoxybenzoate

Space Group: Pbc_a **Cell:** a 7.842(0) b 14.680(0) c 25.768(1)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.68 **Temperature(K):** 296 **Density(g/cm³):** 1.564

Parameters

Fragment 1
ANG1 (Å) 85.921
ANG2 (Å) 48.705
ANG3 (Å) 74.044



EVEVEH

Reference: H.-K.Fun, T.Shahani, B.Garudachari, A.M.Isloor, M.N.Satygarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1802

Formula: C₁₅H₁₁Cl₁O₃

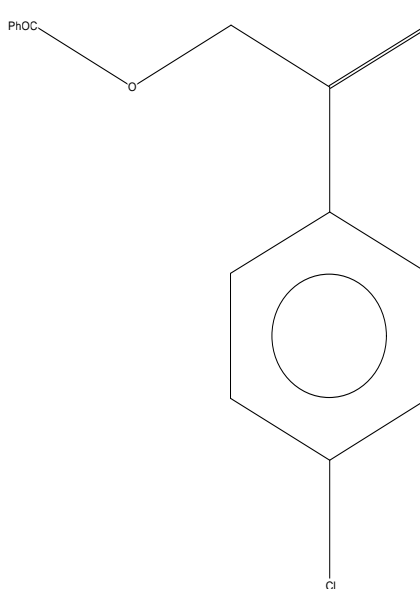
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl benzoate

Space Group: P2₁/c **Cell:** a 8.196(0) b 10.872(1) c 16.542(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 117.82(0) γ 90.00

R-Factor (%): 4.41 **Temperature(K):** 296 **Density(g/cm³):** 1.400

Parameters

Fragment 1
ANG1 (Å) 84.286
ANG2 (Å) 50.331
ANG3 (Å) 65.552



GARCEJ

Reference: A.M.Isloor, B.Garudachari, M.N.Satygarayan, T.Gerber, E.Hosten, R.Betz (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **68**,o513

Formula: C₁₆H₁₃F₁O₄

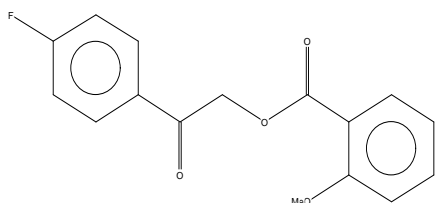
Compound Name: 2-(4-Fluorophenyl)-2-oxoethyl 2-methoxybenzoate

Space Group: P2₁/c **Cell:** a 7.937(0) b 26.446(0) c 7.064(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 113.40(0) γ 90.00

R-Factor (%): 3.73 **Temperature(K):** 200 **Density(g/cm³):** 1.407

Parameters

Fragment 1
ANG1 (Å) 73.676
ANG2 (Å) 45.791
ANG3 (Å) 73.072



GESBUE

Reference: Huirong Zhang, Anuj Kunadia, Yingfu Lin, J.D.Fondell, D.Seidel, Huizhou Fan (2017) *Plos One*, **12**,e0185783

Formula: C₂₁H₁₇N₁O₃

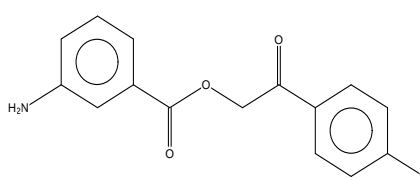
Compound Name: 2-(biphenyl-4-yl)-2-oxoethyl 3-aminobenzoate

Space Group: P-1 **Cell:** a 5.293(0) b 11.682(1) c 13.404(1)
Space Group No.: 2 **(Å, °)** α 87.86(0) β 83.98(0) γ 87.70(0)

R-Factor (%): 5.45 **Temperature(K):** 294 **Density(g/cm³):** 1.337

Parameters

Fragment 1
ANG1 (Å) 75.690
ANG2 (Å) 45.492
ANG3 (Å) 61.521



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 37-40

GITHUN

Reference: Yi Jin, Jian-Nan Guo, Kan Lin, Guo Tang, Yu-Fen Zhao (2008) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **64**,o507

Formula: C₁₅H₁₁Cl₁O₃

Compound Name: Benzoylmethyl 4-chlorobenzoate

Space Group: P21/c **Cell:** a 14.763(0) b 16.451(0) c 15.821(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 92.11(0) γ 90.00

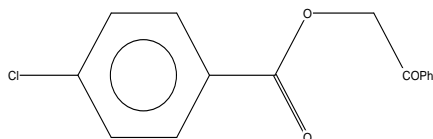
R-Factor (%): 3.65 **Temperature(K):** 293 **Density(g/cm³):** 1.425

Parameters

Fragment 1
ANG1 (A) 77.288
ANG2 (A) 43.515
ANG3 (A) 66.107

Fragment 2
ANG1 (A) 61.687
ANG2 (A) 36.913
ANG3 (A) 58.896

Fragment 3
ANG1 (A) 77.666
ANG2 (A) 47.925
ANG3 (A) 73.608



IDIWID

Reference: B.Garudachari, A.M.Isloor, T.Gerber, E.Hosten, R.Betz (2013) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **69**,o649

Formula: C₁₉H₁₃Br₁O₃

Compound Name: 2-(4-Bromophenyl)-2-oxoethyl naphthalene-1-carboxylate

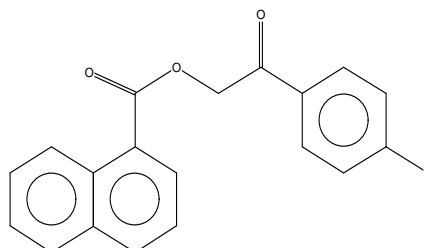
Synonym: 2-(4-Bromophenyl)-2-oxoethyl 1-naphthoate

Space Group: P21/c **Cell:** a 5.289(0) b 14.914(0) c 20.027(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 100.87(0) γ 90.00

R-Factor (%): 3.40 **Temperature(K):** 200 **Density(g/cm³):** 1.581

Parameters

Fragment 1
ANG1 (A) 78.182
ANG2 (A) 60.487
ANG3 (A) 84.596



KULLIO

Reference: Diwaker, C.S.Chidan Kumar, A.Kumar, S.Chandraj, Hoong-Kun Fun, Ching Kheng Quah (2015) *J.Mol.Struct.*, **1092**,192

Formula: C₁₆H₁₃Br₁O₃

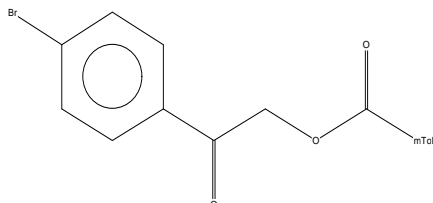
Compound Name: 2-(4-bromophenyl)-2-oxoethyl 3-methylbenzoate

Space Group: P21/c **Cell:** a 8.176(2) b 7.828(2) c 22.952(6)
Space Group No.: 14 **(Å,°)** α 90.00 β 91.33(0) γ 90.00

R-Factor (%): 4.48 **Temperature(K):** 296 **Density(g/cm³):** 1.507

Parameters

Fragment 1
ANG1 (A) 86.034
ANG2 (A) 57.191
ANG3 (A) 74.641



MANGIR

Reference: I.V.Komarov, M.V.Gorichko, O.V.Shishkin, M.Yu.Kornilov (1999) *Zh.Org.Khim.(Russ.)(Russ.J.Org.Chem.)*, **35**,1416

Formula: C₁₈H₁₇Br₁O₃

Compound Name: Phenacyl 5-bromo-2,3,4-trimethylbenzoate

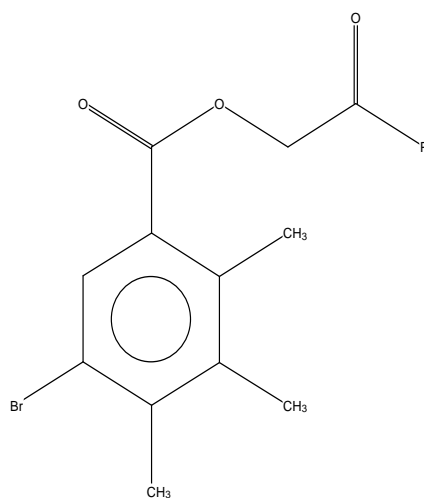
Space Group: P-1 **Cell:** a 10.200(6) b 10.338(4) c 16.110(7)
Space Group No.: 2 **(Å,°)** α 90.63(1) β 93.11(1) γ 97.49(1)

R-Factor (%): 7.07 **Temperature(K):** 295 **Density(g/cm³):** 1.427

Parameters

Fragment 1
ANG1 (A) 70.746
ANG2 (A) 61.014
ANG3 (A) 60.463

Fragment 2
ANG1 (A) 77.848
ANG2 (A) 57.899
ANG3 (A) 67.499



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 41-44

OBOYIP

Reference: H.-K.Fun, T.Shahani, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3154

Formula: C₁₆H₁₃Br₁O₃

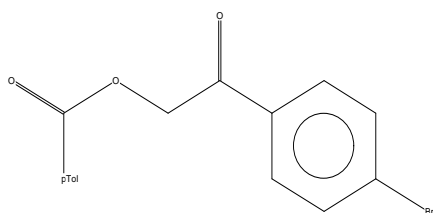
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-methylbenzoate

Space Group: P2₁/c **Cell:** a 5.837(0) b 8.344(0) c 27.968(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.18(0) γ 90.00

R-Factor (%): 2.81 **Temperature(K):** 100 **Density(g/cm³):** 1.631

Parameters

Fragment 1
ANG1 (A) 80.594
ANG2 (A) 42.955
ANG3 (A) 69.145



OCAKUA

Reference: H.-K.Fun, C.K.Quah, A.M.Vijesh, A.M.Isloor, T.Arulmoli (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3351

Formula: C₁₇H₁₅Cl₁O₅

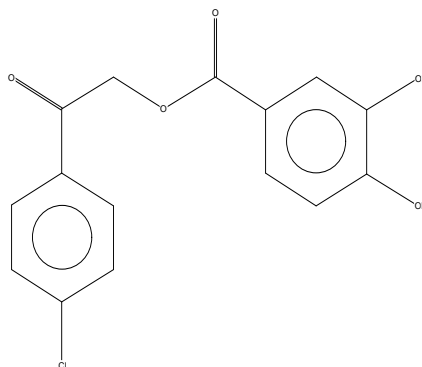
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 3,4-dimethoxybenzoate

Space Group: P-1 **Cell:** a 8.228(0) b 9.338(0) c 10.599(0)
Space Group No.: 2 **(Å, °)** α 89.06(0) β 76.75(0) γ 83.67(0)

R-Factor (%): 5.20 **Temperature(K):** 296 **Density(g/cm³):** 1.411

Parameters

Fragment 1
ANG1 (A) 74.449
ANG2 (A) 52.177
ANG3 (A) 64.990



OCAQUG

Reference: H.-K.Fun, T.S.Chia, S.Shenvi, A.M.Isloor, B.Garudachari (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3379

Formula: C₁₆H₁₂Cl₂O₄

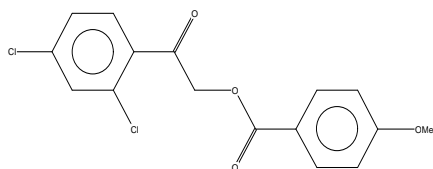
Compound Name: 2-(2,4-Dichlorophenyl)-2-oxoethyl 4-methoxybenzoate

Space Group: P2₁/c **Cell:** a 9.051(0) b 7.085(0) c 23.334(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 102.51(0) γ 90.00

R-Factor (%): 3.89 **Temperature(K):** 100 **Density(g/cm³):** 1.542

Parameters

Fragment 1
ANG1 (A) 70.108
ANG2 (A) 49.241
ANG3 (A) 80.999



OCEFEJ

Reference: H.-K.Fun, W.-S.Loh, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3456

Formula: C₁₆H₁₃F₁O₄

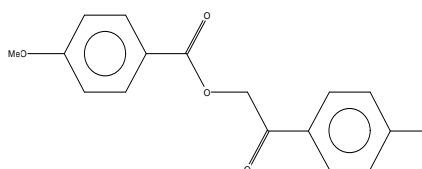
Compound Name: 2-(4-Fluorophenyl)-2-oxoethyl 4-methoxybenzoate

Space Group: P2₁/c **Cell:** a 9.352(0) b 10.195(0) c 15.647(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 118.84(0) γ 90.00

R-Factor (%): 5.49 **Temperature(K):** 100 **Density(g/cm³):** 1.465

Parameters

Fragment 1
ANG1 (A) 84.275
ANG2 (A) 44.601
ANG3 (A) 80.665



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 45-48

PAXCOI

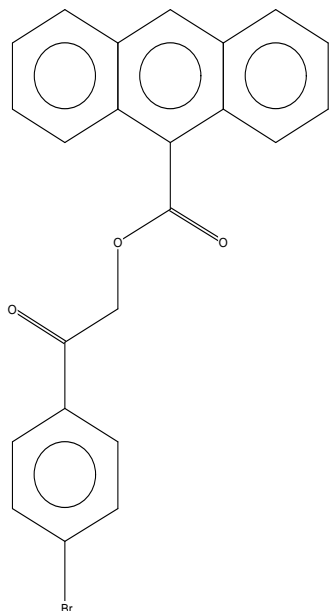
Reference: H.-K.Fun, S.I.J.Asik, B.Garudachari, A.M.Isloor, M.Satyanarayan (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,68, o1876

Formula: C₂₃H₁₅Br₁O₃

Compound Name: 2-(4-Bromophenyl)-2-oxoethyl anthracene-9-carboxylate

Space Group: P21/c **Cell:** a 10.191(0) b 15.059(1) c 13.794(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 122.38(0) γ 90.00

R-Factor (%): 4.52 **Temperature(K):** 100 **Density(g/cm³):** 1.558



Parameters
Fragment 1
ANG1 (A) 5.499
ANG2 (A) 59.667
ANG3 (A) 63.073

PECZAA

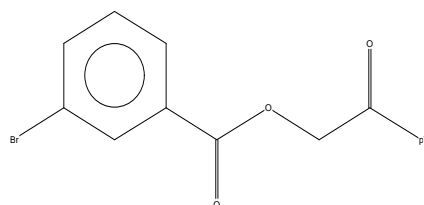
Reference: I.Khan, A.Ibrar, A.Korzanski, M.Kubicki (2012) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,68,o3465

Formula: C₁₆H₁₃Br₁O₃

Compound Name: 2-(4-Methylphenyl)-2-oxoethyl 3-bromobenzoate

Space Group: P-1 **Cell:** a 4.798(0) b 10.995(0) c 14.165(0)
Space Group No.: 2 **(Å, °)** α 74.83(0) β 87.76(0) γ 79.33(0)

R-Factor (%): 3.78 **Temperature(K):** 295 **Density(g/cm³):** 1.561



Parameters
Fragment 1
ANG1 (A) 46.173
ANG2 (A) 19.889
ANG3 (A) 27.092

PODQIK

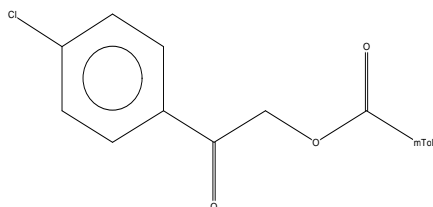
Reference: C.S.Chidan Kumar, C.Yohannan Panicker, Hoong-Kun Fun, Y.Sheena Mary, B.Harikumar, S.Chandraju, Ching Kheng Quah, Chin Wei Ooi (2014) *Spectrochim.Acta, Part A* , 128,327

Formula: C₁₆H₁₃Cl₁O₃

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

Space Group: P21/c **Cell:** a 4.744(0) b 29.316(5) c 10.421(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 92.76(0) γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 297 **Density(g/cm³):** 1.325



Parameters
Fragment 1
ANG1 (A) 67.811
ANG2 (A) 51.421
ANG3 (A) 80.526

PODRAD

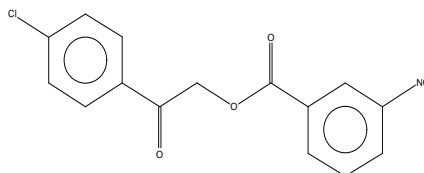
Reference: C.S.Chidan Kumar, C.Yohannan Panicker, Hoong-Kun Fun, Y.Sheena Mary, B.Harikumar, S.Chandraju, Ching Kheng Quah, Chin Wei Ooi (2014) *Spectrochim.Acta, Part A* , 126,208

Formula: C₁₅H₁₀Cl₁N₁O₅

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

Search: search1 (Sun Oct 13 16:24:06 2019): Hits 49-52

QIKVAH

Reference: Y.Kashiwada, K.Yamazaki, Y.Ikeshiro, T.Yamagishi, T.Fujioka, K.Mihashi, K.Mizuki, L.M.Cosentino, K.Fowke, S.L.Morris-Natschke, Kuo-Hsiung Lee (2001) *Tetrahedron*, **57**,1559

Formula: C₃₁ H₃₅ Br₁ O₅

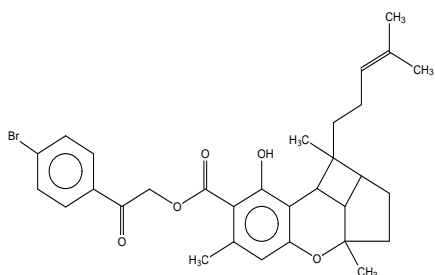
Compound Name: p-Bromophenacyl rhododaurichromanoid acid A

Space Group: P21 **Cell:** a 8.505(2) b 27.809(0) c 5.901(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 95.32(2) γ 90.00

R-Factor (%): 3.59 **Temperature(K):** 295 **Density(g/cm³):** 1.356

Parameters

Fragment 1
ANG1 (A) 89.757
ANG2 (A) 50.849
ANG3 (A) 76.771



USIWID

Reference: H.-K.Fun, S.Arshad, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1528

Formula: C₁₅ H₁₂ O₃

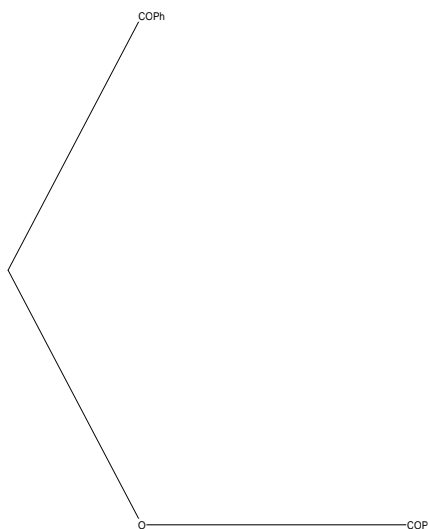
Compound Name: 2-Oxo-2-phenylethyl benzoate

Space Group: P21/c **Cell:** a 9.030(1) b 14.116(2) c 9.638(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.56(0) γ 90.00

R-Factor (%): 5.97 **Temperature(K):** 296 **Density(g/cm³):** 1.299

Parameters

Fragment 1
ANG1 (A) 86.092
ANG2 (A) 67.451
ANG3 (A) 56.918



USIWID01

Reference: S.Khamarui, R.Maiti, D.K.Maiti (2015) *Chem.Commun.*, **51**, 384

Formula: C₁₅ H₁₂ O₃

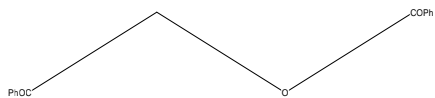
Compound Name: 2-Oxo-2-phenylethyl benzoate

Space Group: P21/c **Cell:** a 9.016(1) b 14.112(2) c 9.680(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.55(0) γ 90.00

R-Factor (%): 6.96 **Temperature(K):** 296 **Density(g/cm³):** 1.296

Parameters

Fragment 1
ANG1 (A) 85.431
ANG2 (A) 67.111
ANG3 (A) 56.679



USIWID02

Reference: Meng-Yang Chang (2016) *CSD Communication(Private Communication)*,

Formula: C₁₅ H₁₂ O₃

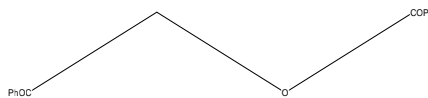
Compound Name: 2-oxo-2-phenylethyl benzoate

Space Group: P21/c **Cell:** a 9.067(0) b 14.127(0) c 9.608(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 90.78(0) γ 90.00

R-Factor (%): 4.46 **Temperature(K):** 296 **Density(g/cm³):** 1.297

Parameters

Fragment 1
ANG1 (A) 86.592
ANG2 (A) 67.891
ANG3 (A) 57.034



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 53-56

USIWOJ

Reference: H.-K.Fun, W.-S.Loh, B.Garudachari, A.M.Isloor, M.N.Satyanarayan (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o1529

Formula: C₁₆H₁₃Br₁O₄

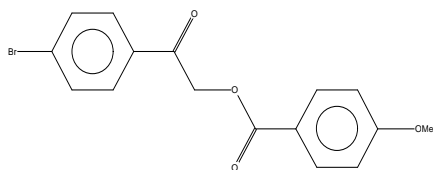
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-methoxybenzoate

Space Group: P-1 **Cell:** a 7.970(0) b 7.985(0) c 11.319(0)
Space Group No.: 2 **(Å, °)** α 86.54(0) β 83.20(0) γ 89.63(0)

R-Factor (%): 2.65 **Temperature(K):** 296 **Density(g/cm³):** 1.624

Parameters

Fragment 1
ANG1 (A) 84.066
ANG2 (A) 58.224
ANG3 (A) 80.862



VOBYUI

Reference: C.S.Chidan Kumar, Hoong Kun Fun, M.Tursun, Chin Wei Ooi, S.Chandrasekar, Ching Kheng Quah, C.Parlak (2014) *Spectrochim.Acta, Part A*, **124**,595

Formula: C₁₅H₁₀Cl₂O₃

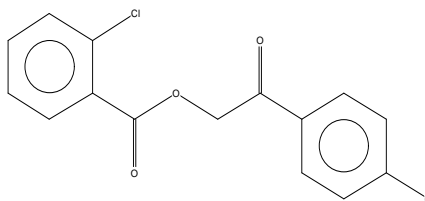
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 2-chlorobenzoate

Space Group: Pbc_a **Cell:** a 12.312(5) b 8.103(3) c 27.565(11)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.71 **Temperature(K):** 293 **Density(g/cm³):** 1.493

Parameters

Fragment 1
ANG1 (A) 5.954
ANG2 (A) 5.773
ANG3 (A) 1.689



WIGTUD

Reference: B.Garudachari, A.M.Isloor, T.Gerber, E.Hosten, R.Betz (2013) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **69**,o551

Formula: C₁₉H₁₃Cl₁O₃

Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl naphthalene-1-carboxylate

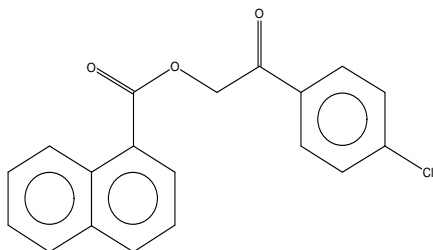
Synonym: 2-(4-Chlorophenyl)-2-oxoethyl 1-naphthoate

Space Group: P2₁/c **Cell:** a 5.271(0) b 14.847(0) c 19.843(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.38(0) γ 90.00

R-Factor (%): 3.54 **Temperature(K):** 200 **Density(g/cm³):** 1.412

Parameters

Fragment 1
ANG1 (A) 78.056
ANG2 (A) 60.249
ANG3 (A) 84.496



YAFWEJ

Reference: H.-K.Fun, S.Arshad, B.Garudachari, A.M.Isloor, K.N.Shivananda (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**, o2836

Formula: C₁₆H₁₀F₄O₃

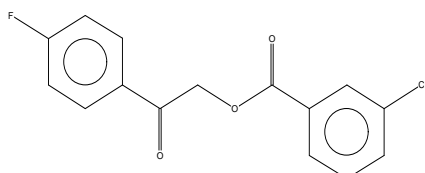
Compound Name: 2-(4-Fluorophenyl)-2-oxoethyl 3-(trifluoromethyl)benzoate

Space Group: P2₁/c **Cell:** a 14.769(1) b 12.160(1) c 8.093(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.89(0) γ 90.00

R-Factor (%): 5.74 **Temperature(K):** 296 **Density(g/cm³):** 1.499

Parameters

Fragment 1
ANG1 (A) 20.336
ANG2 (A) 5.349
ANG3 (A) 17.215



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 57-60

YAFZAI

Reference: H.-K.Fun, W.-S.Loh, B.Garudachari, A.M.Isloor, M.N.Satyanarayana (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o2854

Formula: C₁₅H₁₁Br₁O₄

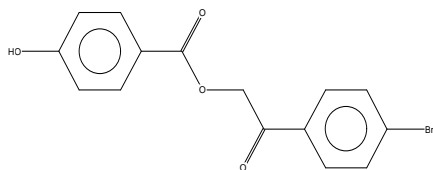
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 4-hydroxybenzoate

Space Group: P21/c **Cell:** a 6.292(0) b 7.789(0) c 26.750(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 98.23(0) γ 90.00

R-Factor (%): 3.36 **Temperature(K):** 100 **Density(g/cm³):** 1.716

Parameters

Fragment 1
ANG1 (Å) 66.766
ANG2 (Å) 44.992
ANG3 (Å) 56.390



YAHGUL

Reference: H.-K.Fun, W.-S.Loh, B.Garudachari, A.M.Isloor, M.N.Satyanarayana (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3030

Formula: C₁₆H₁₃Cl₁O₃

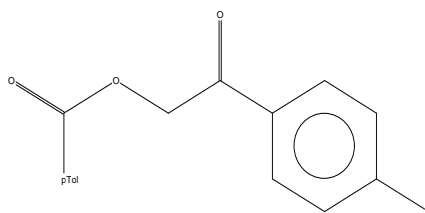
Compound Name: 2-(4-Chlorophenyl)-2-oxoethyl 4-methylbenzoate

Space Group: P21/c **Cell:** a 5.913(0) b 8.504(0) c 27.877(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 95.88(0) γ 90.00

R-Factor (%): 4.60 **Temperature(K):** 297 **Density(g/cm³):** 1.375

Parameters

Fragment 1
ANG1 (Å) 80.735
ANG2 (Å) 44.446
ANG3 (Å) 68.625



YAHYOX

Reference: H.-K.Fun, C.W.Ooi, B.Garudachari, A.M.Isloor, M.N.Satyanarayana (2011) *Acta Crystallogr., Sect.E:Struct.Rep.Online*, **67**,o3119

Formula: C₁₆H₁₃Br₁O₃

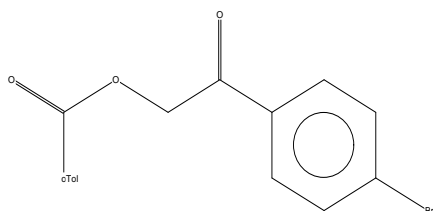
Compound Name: 2-(4-Bromophenyl)-2-oxoethyl 2-methylbenzoate

Space Group: P21/c **Cell:** a 5.452(0) b 31.238(0) c 9.721(0)
Space Group No.: 14 **(Å, °)** α 90.00 β 120.41(0) γ 90.00

R-Factor (%): 4.01 **Temperature(K):** 100 **Density(g/cm³):** 1.550

Parameters

Fragment 1
ANG1 (Å) 66.659
ANG2 (Å) 52.766
ANG3 (Å) 87.307



ZARCED

Reference: S.Kumar, Chandra, B.M.Rajesh, M.Mahendra, B.H.Doreswamy (2017) *IUCrData*, **2**,x170183

Formula: C₁₈H₁₈O₅

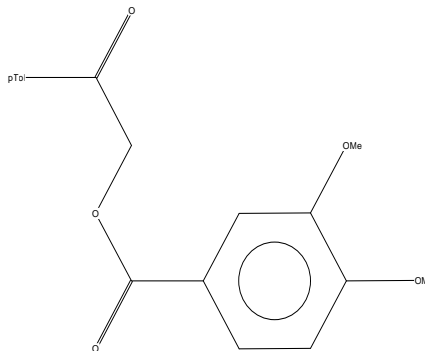
Compound Name: 2-(4-methylphenyl)-2-oxoethyl 3,4-dimethoxybenzoate

Space Group: P-1 **Cell:** a 7.981(0) b 8.609(0) c 11.467(0)
Space Group No.: 2 **(Å, °)** α 99.68(0) β 99.17(0) γ 91.50(0)

R-Factor (%): 4.57 **Temperature(K):** 293 **Density(g/cm³):** 1.364

Parameters

Fragment 1
ANG1 (Å) 66.545
ANG2 (Å) 42.982
ANG3 (Å) 87.728



Search: search1 (Sun Oct 13 16:24:06 2019): Hits 61-62

POCGAS

Reference: Taoshan Xu, Chaoxian Yan, Yuewei Wu, Chengshan Yuan, Xiangfeng Shao (2019) *Dyes Pigm.* ,168,235

Formula: C₁₆ H₁₂ Cl₂ O₄

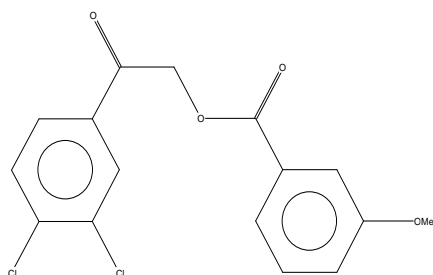
Compound Name: 2-(3,4-dichlorophenyl)-2-oxoethyl 3-methoxybenzoate

Space Group: P2₁/c **Cell:** **a** 4.262(1) **b** 31.860(10) **c** 11.222(4)
Space Group No.: 14 **(Å, °)** **α** 90.00 **β** 101.92(1) **γ** 90.00

R-Factor (%): 5.84 **Temperature(K):** 296 **Density(g/cm³):** 1.511

Parameters

Fragment 1
ANG1 (A) 37.702
ANG2 (A) 18.527
ANG3 (A) 19.405



POCGEW

Reference: Taoshan Xu, Chaoxian Yan, Yuewei Wu, Chengshan Yuan, Xiangfeng Shao (2019) *Dyes Pigm.* ,168,235

Formula: C₁₆ H₁₂ Cl₂ O₄

Compound Name: 2-(3,4-dichlorophenyl)-2-oxoethyl 4-methoxybenzoate

Space Group: Pbc_a **Cell:** **a** 20.447(3) **b** 8.989(1) **c** 32.705(5)
Space Group No.: 61 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 5.08 **Temperature(K):** 296 **Density(g/cm³):** 1.499

Parameters

Fragment 1
ANG1 (A) 76.546
ANG2 (A) 51.387
ANG3 (A) 63.163

Fragment 2
ANG1 (A) 85.838
ANG2 (A) 57.137
ANG3 (A) 67.767

