

Search Overview

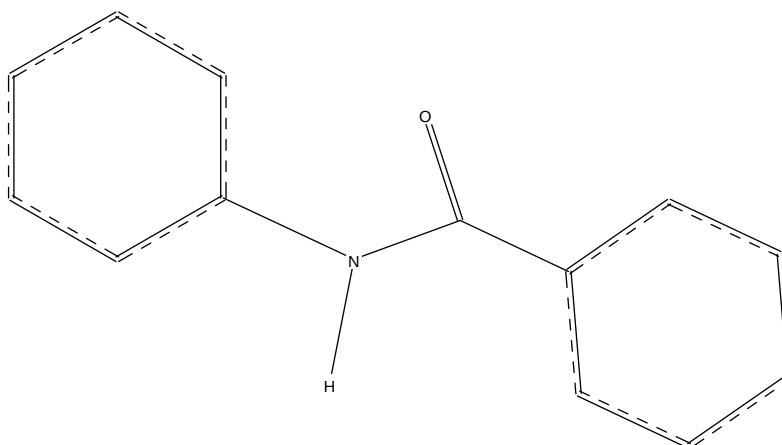
Search:	search1
Date/Time done:	Sun Feb 03 13:27:04 2013
Database(s):	CSD version 5.34 updates (Nov 2012) CSD version 5.34 (November 2012)
Restriction Info:	No refcode restrictions applied
Filters:	None
Percentage Completed:	100%
Number of Hits:	1056

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 1-4

AWEWAB

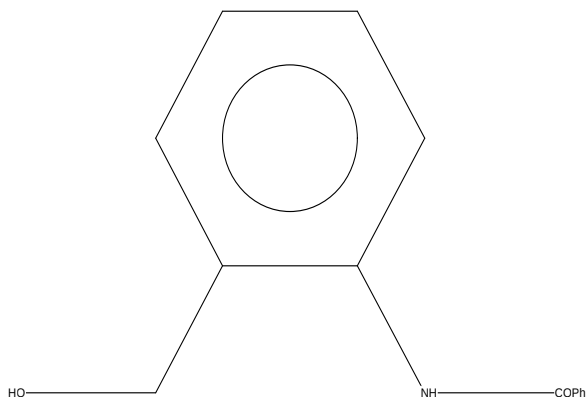
Reference: C.F.Zipp, M.A.Fernandes, H.M.Marques, J.P.Michael, C.B.Perry (2011) *Cryst.Growth Des.* ,**11**,1431

Formula: C₁₄ H₁₃ N₁ O₂

Compound Name: N-(2-(Hydroxymethyl)phenyl)benzamide

Space Group: P2₁/n **Cell:** *a* 12.512(0) *b* 7.327(0) *c* 12.665(0)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 100.05(0) *γ* 90.00

R-Factor (%): 4.17 **Temperature(K):** 173 **Density(g/cm³):** 1.320



AWEWAB01

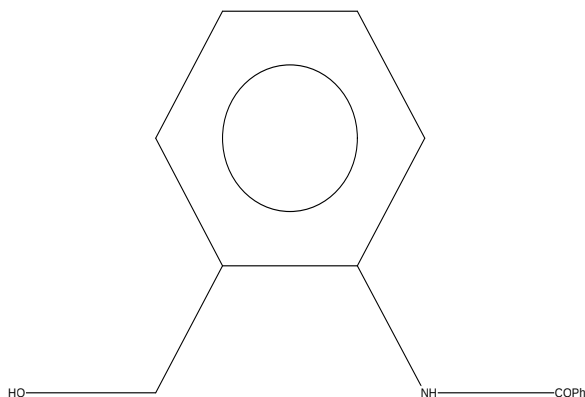
Reference: C.F.Zipp, M.A.Fernandes, H.M.Marques, J.P.Michael, C.B.Perry (2011) *Cryst.Growth Des.* ,**11**,1431

Formula: C₁₄ H₁₃ N₁ O₂

Compound Name: N-(2-(Hydroxymethyl)phenyl)benzamide

Space Group: P2₁/n **Cell:** *a* 5.194(0) *b* 13.233(1) *c* 17.032(1)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 90.13(0) *γ* 90.00

R-Factor (%): 5.55 **Temperature(K):** 173 **Density(g/cm³):** 1.290



BZANIL

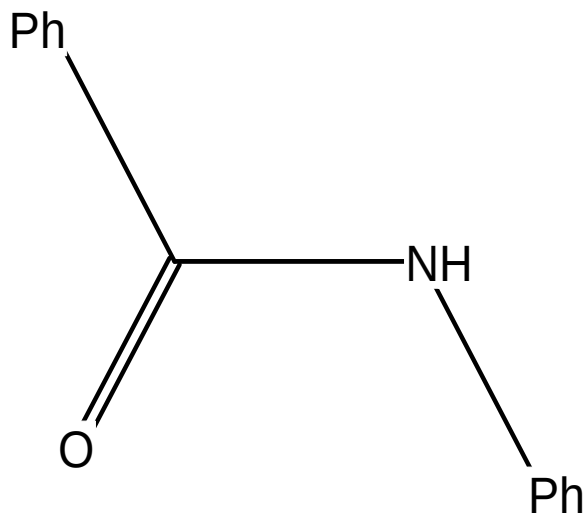
Reference: S.Kashino, K.Ito, M.Haisa (1979) *Bull.Chem.Soc.Jpn.* ,**52**, 365

Formula: C₁₃ H₁₁ N₁ O₁

Compound Name: N-Benzoylaniline

Space Group: C2/c **Cell:** *a* 24.340(40) *b* 5.325(3) *c* 8.012(8)
Space Group No.: 15 **Cell:** (*Å*,°) *α* 90.00 *β* 107.20(30) *γ* 90.00

R-Factor (%): 7.50 **Temperature(K):** 295 **Density(g/cm³):** 1.321



BZANIL01

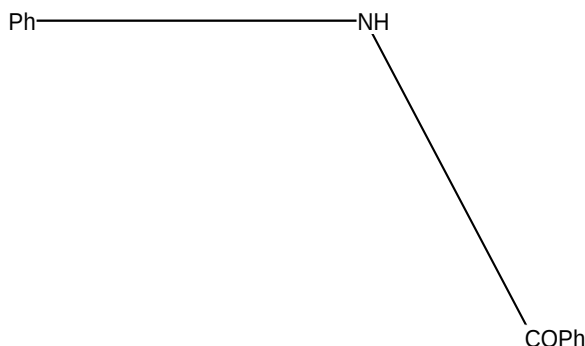
Reference: K.F.Bowes, C.Gliddewell, J.N.Low, J.M.S.Skackle, J.L.Wardell (2003) *Acta Crystallogr., Sect.C:Cryst.Struct. Commun.* ,**59**, o1

Formula: C₁₃ H₁₁ N₁ O₁

Compound Name: N-Benzoylaniline

Space Group: P-1 **Cell:** *a* 5.341(0) *b* 7.773(0) *c* 12.390(1)
Space Group No.: 2 **Cell:** (*Å*,°) *α* 72.70(0) *β* 79.39(0) *γ* 89.91(0)

R-Factor (%): 6.10 **Temperature(K):** 120 **Density(g/cm³):** 1.359



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 5-8

CIYXAK

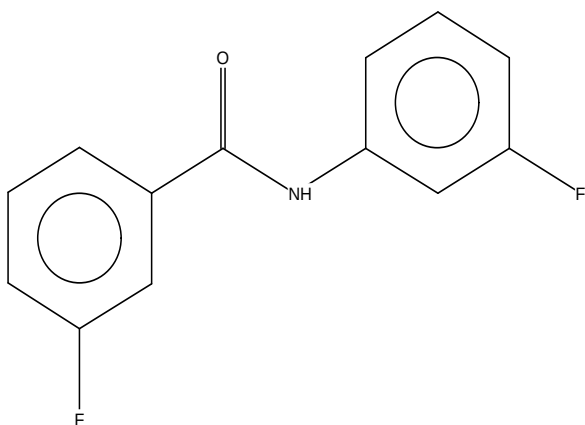
Reference: D.Chopra, T.N.G.Row (2008) *Cryst.Growth Des.* ,8,848

Formula: C₁₃ H₉ F₂ N₁ O₁

Compound Name: 3-Fluoro-N-(3-fluorophenyl)benzamide

Space Group: P2₁ **Cell:** **a** 5.067(0) **b** 5.354(0) **c** 19.302(3)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 95.51(0) **γ** 90.00

R-Factor (%): 6.10 **Temperature(K)**: 100 **Density(g/cm³)**: 1.486



CIYXAK01

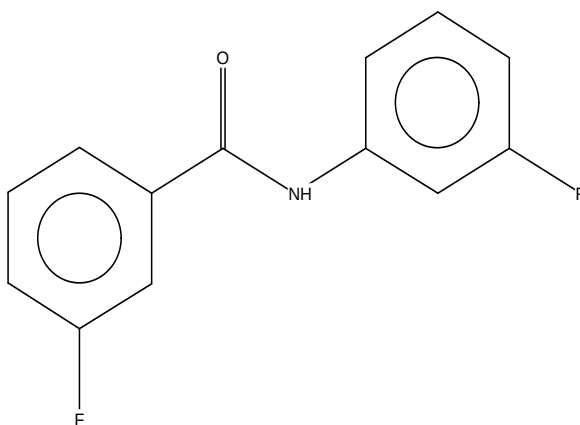
Reference: D.Chopra, T.N.G.Row (2008) *Cryst.Growth Des.* ,8,848

Formula: C₁₃ H₉ F₂ N₁ O₁

Compound Name: 3-Fluoro-N-(3-fluorophenyl)benzamide

Space Group: C2/c **Cell:** **a** 25.242(5) **b** 5.386(1) **c** 8.203(1)
Space Group No.: 15 **(Å,°)** **α** 90.00 **β** 108.14(0) **γ** 90.00

R-Factor (%): 6.21 **Temperature(K)**: 290 **Density(g/cm³)**: 1.462



DIBDEY

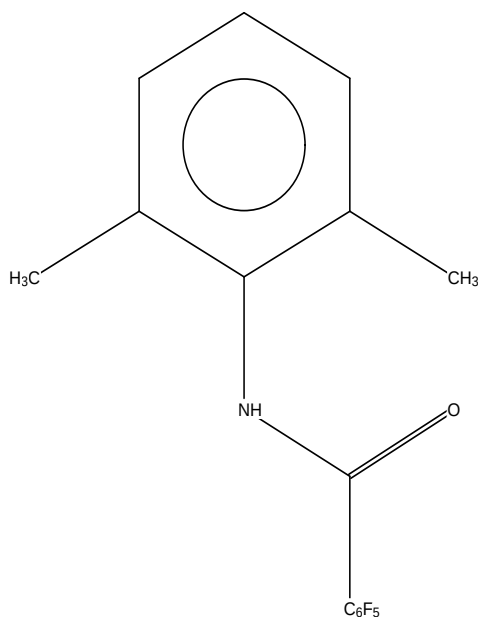
Reference: S.L.Cockroft, J.Perkins, C.Zonta, H.Adams, S.E.Spey, C.M.R.Low, J.G.Vinter, K.R.Lawson, C.J.Urch, C.A.Hunter (2007) *Org.Biomol.Chem.* ,5,1062

Formula: C₁₅ H₁₀ F₅ N₁ O₁

Compound Name: N-(2,6-Dimethylphenyl)-2,3,4,5,6-pentafluorobenzamide

Space Group: P2₁/c **Cell:** **a** 4.750(1) **b** 10.856(2) **c** 26.289(6)
Space Group No.: 14 **(Å,°)** **α** 90.00 **β** 92.26(0) **γ** 90.00

R-Factor (%): 4.35 **Temperature(K)**: 150 **Density(g/cm³)**: 1.546



DIBDEY01

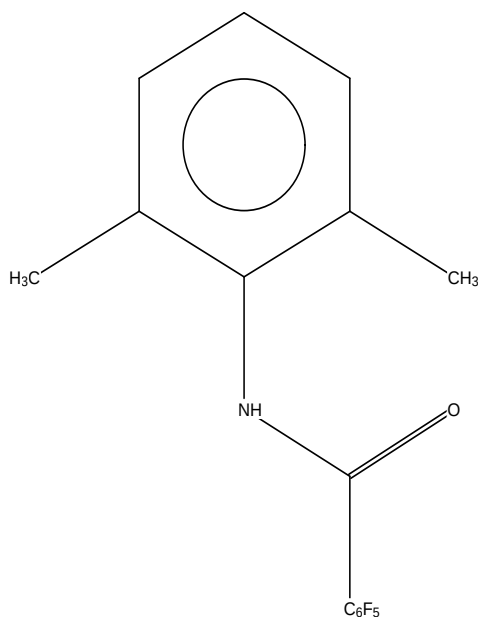
Reference: S.L.Cockroft, J.Perkins, C.Zonta, H.Adams, S.E.Spey, C.M.R.Low, J.G.Vinter, K.R.Lawson, C.J.Urch, C.A.Hunter (2007) *Org.Biomol.Chem.* ,5,1062

Formula: C₁₅ H₁₀ F₅ N₁ O₁

Compound Name: N-(2,6-Dimethylphenyl)-2,3,4,5,6-pentafluorobenzamide

Space Group: Cc **Cell:** **a** 12.822(4) **b** 11.499(3) **c** 9.804(2)
Space Group No.: 9 **(Å,°)** **α** 90.00 **β** 103.84(2) **γ** 90.00

R-Factor (%): 4.74 **Temperature(K)**: 293 **Density(g/cm³)**: 1.492



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 9-12

FEMMAL

Reference: R.Kunstmann, H.Gerhards, H.Kruse, M.Leven, E.F.Paulus, U.Schacht, K.Schmitt, P.U.Witte (1987) *J.Med.Chem.* , **30**, 798

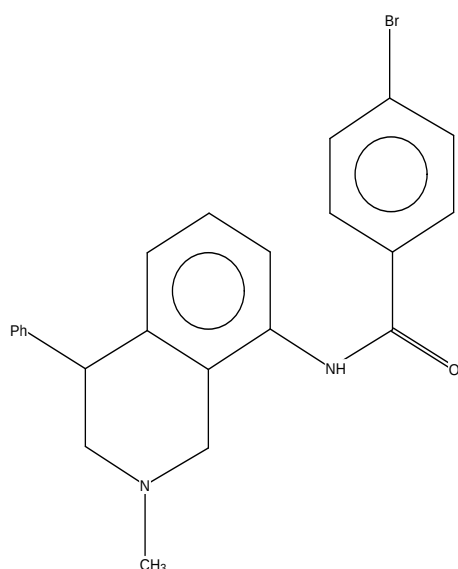
Formula: C₂₃ H₂₁ Br₁ N₂ O₁

Compound Name: (4S)-(+)-8-((4-Bromobenzoyl)amino)-2-methyl-4-phenyl-1,2,3,4-tetrahydro-isoquinoline

Synonym: (4S)-(+)-N-(4-Bromobenzoyl)nomifensine

Space Group: P2₁2₁2₁ **Cell:** **a** 24.680(40) **b** 14.580(20) **c** 5.530(20)
Space Group No.: 19 **Cell:** **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.46 **Temperature(K)**: 295 **Density(g/cm³)**: 1.406



FEMMAL01

Reference: R.Kunstmann, H.Gerhards, H.Kruse, M.Leven, E.F.Paulus, U.Schacht, K.Schmitt, P.U.Witte (1987) *J.Med.Chem.* , **30**, 798

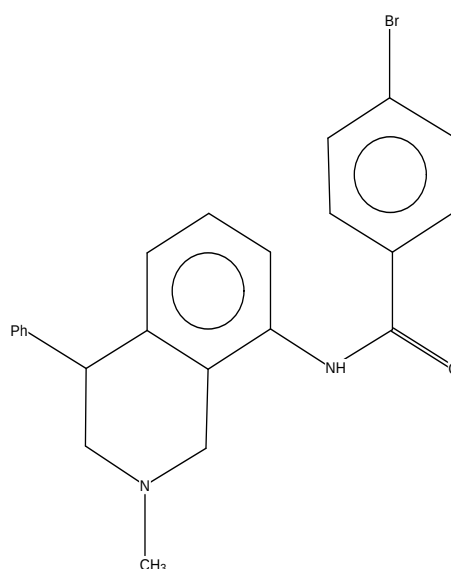
Formula: C₂₃ H₂₁ Br₁ N₂ O₁

Compound Name: (4S)-(+)-8-((4-Bromobenzoyl)amino)-2-methyl-4-phenyl-1,2,3,4-tetrahydro-isoquinoline

Synonym: (4S)-(+)-N-(4-Bromobenzoyl)nomifensine

Space Group: P2₁ **Cell:** **a** 12.224(2) **b** 6.160(1) **c** 13.086(2)
Space Group No.: 4 **Cell:** **(Å,°)** α 90.00 β 92.34(1) γ 90.00

R-Factor (%): 3.47 **Temperature(K)**: 295 **Density(g/cm³)**: 1.421



FENPUJ

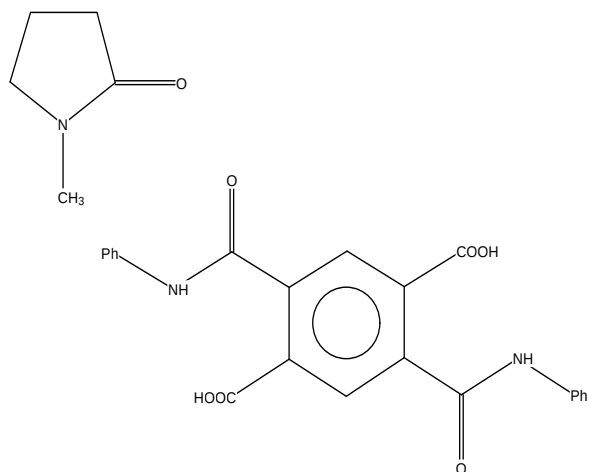
Reference: N.S.Magomedova, L.A.Chetkina, V.K.Bel'skii, Yu.N.Sazanov, S.A.Dauengauer, L.A.Shibaev (1986) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)* , **27**,118-5

Formula: C₂₂ H₁₆ N₂ O₆,2(C₅ H₉ N₁ O₁)

Compound Name: bis(N-Methyl-2-pyrrolidone) pyromellitic acid 1,4-dianilide

Space Group: P-1 **Cell:** **a** 9.701(4) **b** 8.828(4) **c** 10.395(4)
Space Group No.: 2 **Cell:** **(Å,°)** α 84.68(3) β 113.25(3) γ 75.02(3)

R-Factor (%): 4.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.298



FENPUJ01

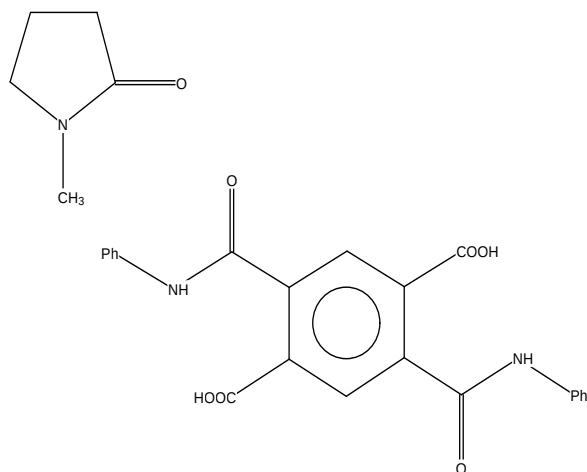
Reference: N.S.Magomedova, L.A.Chetkina, V.K.Bel'skii, Yu.N.Sazanov, S.A.Dauengauer, L.A.Shibaev (1986) *Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.)* , **27**,118-5

Formula: C₂₂ H₁₆ N₂ O₆,2(C₅ H₉ N₁ O₁)

Compound Name: bis(N-Methyl-2-pyrrolidone) pyromellitic acid 1,4-dianilide

Space Group: P1121/b **Cell:** **a** 5.638(2) **b** 9.301(3) **c** 30.366(6)
Space Group No.: 14 **Cell:** **(Å,°)** α 90.00 β 90.00 γ 102.45(3)

R-Factor (%): 10.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.287



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 13-16

GISYOX

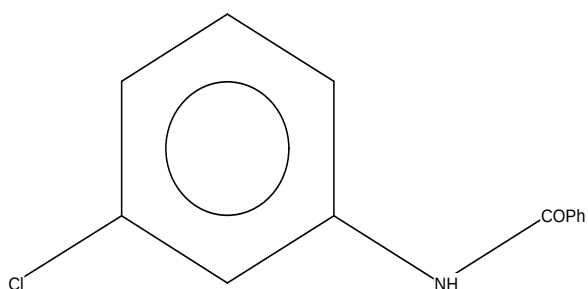
Reference: B.T.Gowda, M.Tokarcik, J.Kozisek, B.P.Sowmya, H.Fuess (2008) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,**64**,o462

Formula: C₁₃ H₁₀ Cl₁ N₁ O₁

Compound Name: N-(3-Chlorophenyl)benzamide

Space Group: Pbc_a **Cell:** **a** 9.359(0) **b** 9.785(0) **c** 25.142(0)
Space Group No.: 61 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.83 **Temperature(K):** 295 **Density(g/cm³):** 1.337



GISYOX01

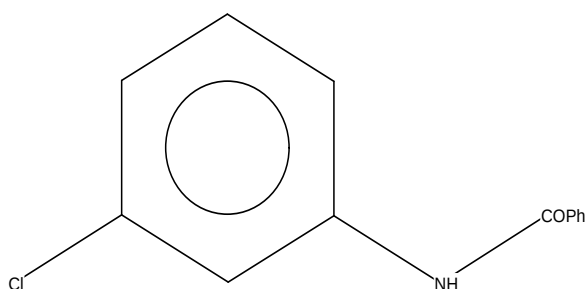
Reference: A.Saeed, M.Arshad, J.Simpson (2010) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,**66**,o2808

Formula: C₁₃ H₁₀ Cl₁ N₁ O₁

Compound Name: N-(3-Chlorophenyl)benzamide

Space Group: P2₁/c **Cell:** **a** 12.560(1) **b** 10.278(1) **c** 9.079(1)
Space Group No.: 14 **(Å, °)** α 90.00 β 109.42(0) γ 90.00

R-Factor (%): 4.05 **Temperature(K):** 90 **Density(g/cm³):** 1.392



INODUK

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2004) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.* ,**60**,o120

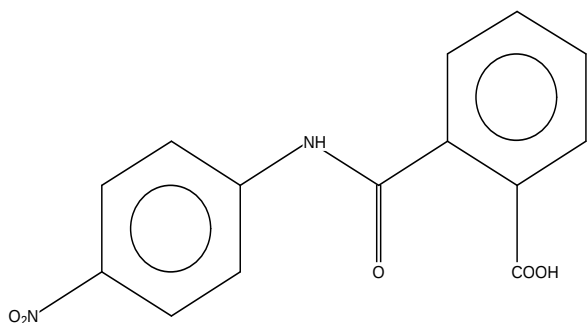
Formula: C₁₄ H₁₀ N₂ O₅

Compound Name: 2-(4-Nitrophenylaminocarbonyl)benzoic acid

Synonym: N-(4-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: P2₁/n **Cell:** **a** 10.210(1) **b** 9.375(0) **c** 27.409(2)
Space Group No.: 14 **(Å, °)** α 90.00 β 100.58(0) γ 90.00

R-Factor (%): 6.90 **Temperature(K):** 120 **Density(g/cm³):** 1.474



INODUK01

Reference: C.Glidewell, J.N.Low, J.M.S.Skakle, J.L.Wardell (2004) *Acta Crystallogr., Sect.C: Cryst. Struct. Commun.* ,**60**,o120

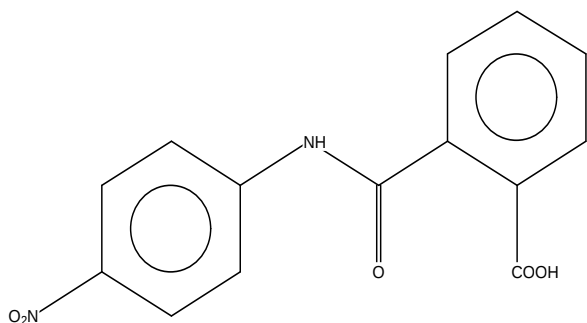
Formula: C₁₄ H₁₀ N₂ O₅

Compound Name: 2-(4-Nitrophenylaminocarbonyl)benzoic acid

Synonym: N-(4-Nitrophenyl)benzamide-2-carboxylic acid

Space Group: P2₁2₁2₁ **Cell:** **a** 3.919(0) **b** 12.690(0) **c** 27.703(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

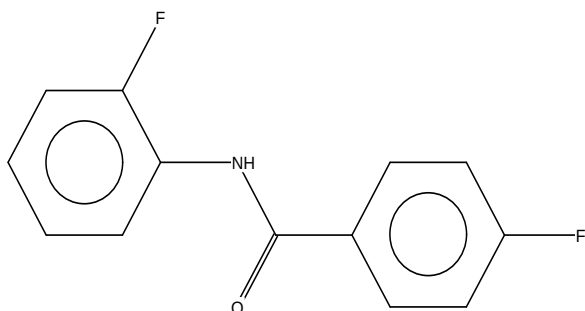
R-Factor (%): 5.50 **Temperature(K):** 120 **Density(g/cm³):** 1.380



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 17-20

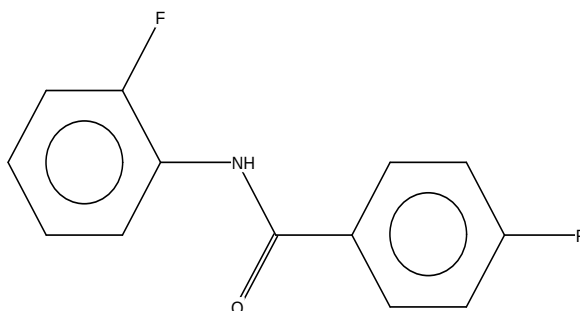
JAVWIN

Reference: D.Chopra, T.N.G.Row (2005) *Cryst.Growth Des.* ,**5**,1679
Formula: C₁₃ H₉ F₂ N₁ O₁
Compound Name: 4-Fluoro-N-(2-fluorophenyl)benzamide
Space Group: Pca21 **Cell:** **a** 25.563(13) **b** 4.969(2) **c** 8.250(4)
Space Group No.: 29 **(Å,°)** **α** 90.00 **β** 90.00 **γ** 90.00
R-Factor (%): 5.45 **Temperature(K)**: 295 **Density(g/cm³)**: 1.478



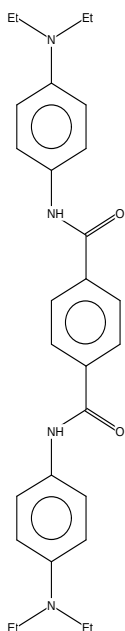
JAVWIN01

Reference: D.Chopra, T.N.G.Row (2005) *Cryst.Growth Des.* ,**5**,1679
Formula: C₁₃ H₉ F₂ N₁ O₁
Compound Name: 4-Fluoro-N-(2-fluorophenyl)benzamide
Space Group: P21 **Cell:** **a** 4.962(1) **b** 5.486(1) **c** 19.174(5)
Space Group No.: 4 **(Å,°)** **α** 90.00 **β** 91.76(0) **γ** 90.00
R-Factor (%): 4.43 **Temperature(K)**: 100 **Density(g/cm³)**: 1.485



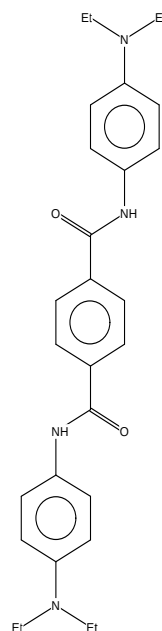
KUQLEO

Reference: P.Kus, J.Borek, P.G.Jones (2010) *Acta Crystallogr.,Sect.C:Cryst.Struct.Comm.* ,**66**,o93
Formula: C₂₈ H₃₄ N₄ O₂
Compound Name: N,N'-bis[4-(diethylamino)phenyl]terephthaldiamide
Space Group: P-1 **Cell:** **a** 5.110(0) **b** 9.946(3) **c** 12.107(3)
Space Group No.: 2 **(Å,°)** **α** 100.54(2) **β** 93.90(2) **γ** 103.53(2)
R-Factor (%): 5.29 **Temperature(K)**: 100 **Density(g/cm³)**: 1.304



KUQLEO01

Reference: P.Kus, J.Borek, P.G.Jones (2010) *Acta Crystallogr.,Sect.C:Cryst.Struct.Comm.* ,**66**,o93
Formula: C₂₈ H₃₄ N₄ O₂
Compound Name: N,N'-bis[4-(Diethylamino)phenyl]terephthaldiamide
Space Group: Cc **Cell:** **a** 11.590(0) **b** 16.790(0) **c** 13.479(0)
Space Group No.: 9 **(Å,°)** **α** 90.00 **β** 114.67(0) **γ** 90.00
R-Factor (%): 5.49 **Temperature(K)**: 100 **Density(g/cm³)**: 1.278



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 21-24

PABZAM

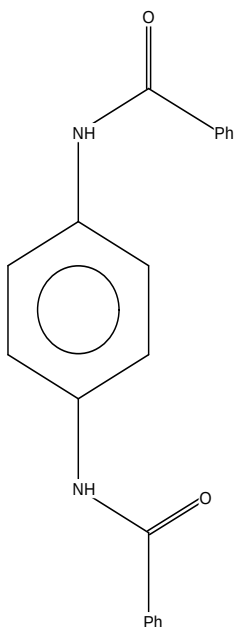
Reference: S.Harkema, R.J.Gaymans (1977)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem., **33**,3609

Formula: C₂₀ H₁₆ N₂ O₂

Compound Name: N,N'-(p-Phenylene)-dibenzamide

Space Group: P2₁/c **Cell:** *a* 18.065(1) *b* 5.247(1) *c* 8.027(1)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 93.99(1) *γ* 90.00

R-Factor (%): 7.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.384



PABZAM01

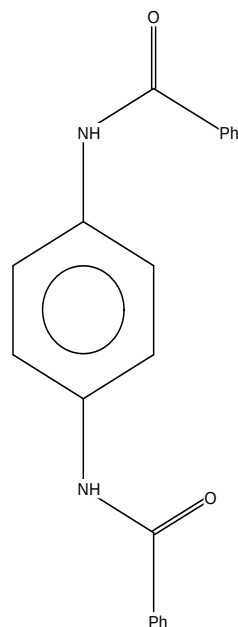
Reference: W.W.Adams, A.V.Fratini, D.R.Wiff (1978)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem., **34**,954

Formula: C₂₀ H₁₆ N₂ O₂

Compound Name: N,N'-Dibenzoyl-p-phenylenediamine

Space Group: Pbca **Cell:** *a* 9.540(7) *b* 18.273(9) *c* 9.387(3)
Space Group No.: 61 **Cell:** (*Å*,°) *α* 90.00 *β* 90.00 *γ* 90.00

R-Factor (%): 8.90 **Temperature(K)**: 295 **Density(g/cm³)**: 1.284



PCHSAN

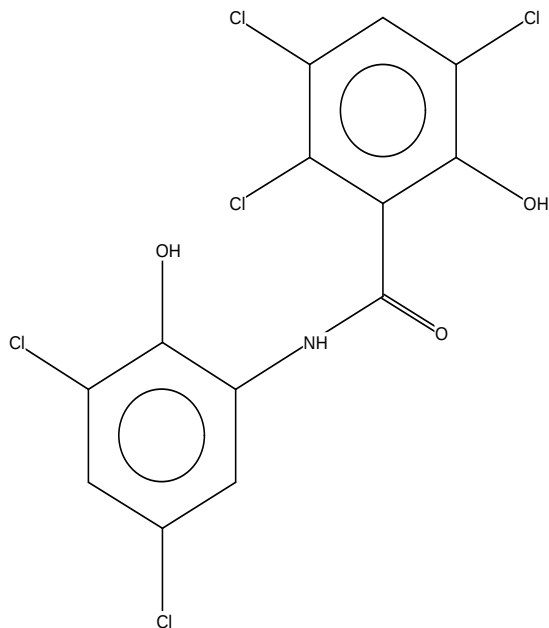
Reference: A.C.Sindt, M.F.Mackay (1979)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem., **35**,2103

Formula: C₁₃ H₆ Cl₅ N₁ O₃

Compound Name: 3,3',5,5',6-Pentachloro-2'-hydroxy-salicylanilide

Space Group: P-1 **Cell:** *a* 8.382(4) *b* 9.392(6) *c* 10.183(3)
Space Group No.: 2 **Cell:** (*Å*,°) *α* 93.06(5) *β* 95.38(3) *γ* 112.61(4)

R-Factor (%): 5.30 **Temperature(K)**: 295 **Density(g/cm³)**: 1.818



PCHSAN01

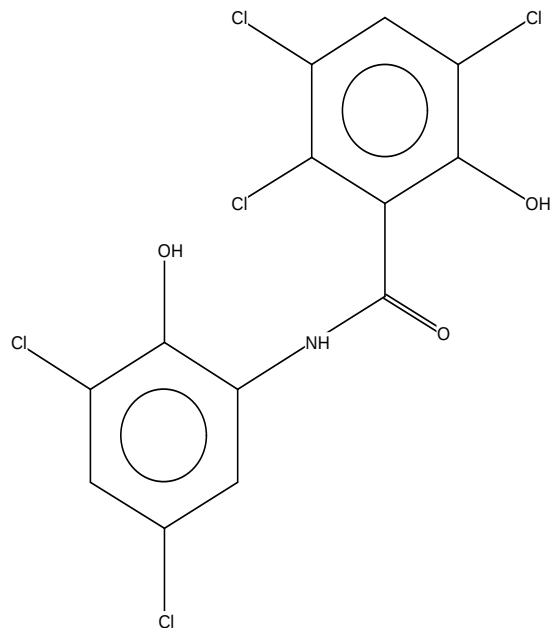
Reference: A.C.Sindt, M.F.Mackay (1979)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem., **35**,2103

Formula: C₁₃ H₆ Cl₅ N₁ O₃

Compound Name: 3,3',5,5',6-Pentachloro-2'-hydroxy-salicylanilide

Space Group: P2₁/n **Cell:** *a* 7.078(6) *b* 23.533(3) *c* 9.359(3)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 110.02(4) *γ* 90.00

R-Factor (%): 6.00 **Temperature(K)**: 295 **Density(g/cm³)**: 1.821



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 25-28

PIWBUT

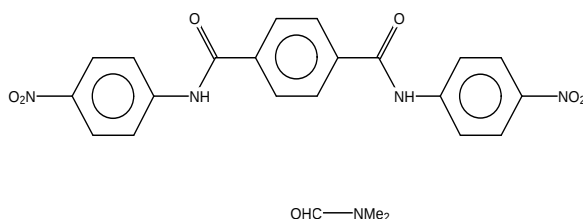
Reference: H.Mehenni, H.Guillou, C.Tessier, J.Brisson (2008)
Can.J.Chem. ,**86**,7

Formula: C₂₀ H₁₄ N₄ O₆.2(C₃ H₇ N₁ O₁)

Compound Name: N,N'-bis(4-Nitrophenyl)benzene-1,4-dicarboxamide dimethylformamide solvate

Space Group: P-1 **Cell:** **a** 10.949(5) **b** 11.918(5) **c** 11.976(5)
Space Group No.: 2 **(Å,°)** α 92.39(0) β 114.71(0) γ 110.84(0)

R-Factor (%): 4.71 **Temperature(K)**: 200 **Density(g/cm³)**: 1.419



PIWBUT01

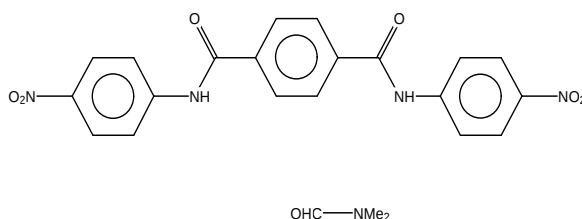
Reference: H.Mehenni, H.Guillou, C.Tessier, J.Brisson (2008)
Can.J.Chem. ,**86**,7

Formula: C₂₀ H₁₄ N₄ O₆.2(C₃ H₇ N₁ O₁)

Compound Name: N,N'-bis(4-Nitrophenyl)benzene-1,4-dicarboxamide dimethylformamide solvate

Space Group: P21/n **Cell:** **a** 3.871(0) **b** 33.189(7) **c** 10.451(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 97.82(0) γ 90.00

R-Factor (%): 4.06 **Temperature(K)**: 294 **Density(g/cm³)**: 1.380



PULHUZ

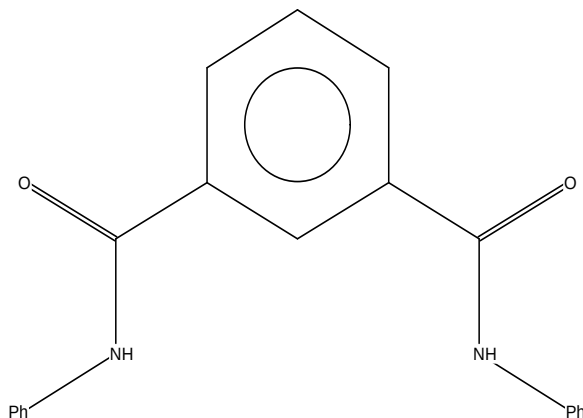
Reference: J.F.Malone, C.M.Murray, G.M.Dolan, R.Docherty, A.J.Lavery (1997) *Chem.Mater.* ,**9**,2983

Formula: C₂₀ H₁₆ N₂ O₂

Compound Name: N,N'-Diphenylisophthalamide

Space Group: Cc **Cell:** **a** 11.827(2) **b** 11.828(2) **c** 23.211(2)
Space Group No.: 9 **(Å,°)** α 90.00 β 102.89(1) γ 90.00

R-Factor (%): 11.91 **Temperature(K)**: 295 **Density(g/cm³)**: 1.328



PULHUZ01

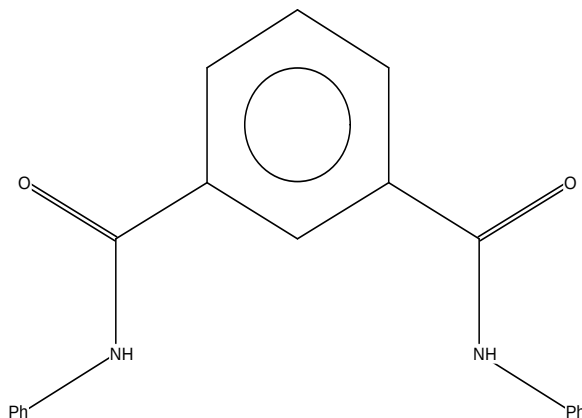
Reference: P.Nimmanpipug, K.Tashiro, Y.Maeda, O.Rangsiman (2002) *J.Phys.Chem.B* ,**106**,6842

Formula: C₂₀ H₁₆ N₂ O₂

Compound Name: N,N'-Diphenylisophthalamide

Space Group: P1 **Cell:** **a** 8.363(0) **b** 8.370(0) **c** 23.387(1)
Space Group No.: 1 **(Å,°)** α 98.90(0) β 101.59(0) γ 90.00(0)

R-Factor (%): 9.50 **Temperature(K)**: 298 **Density(g/cm³)**: 1.327



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 29-32

QUKVUN

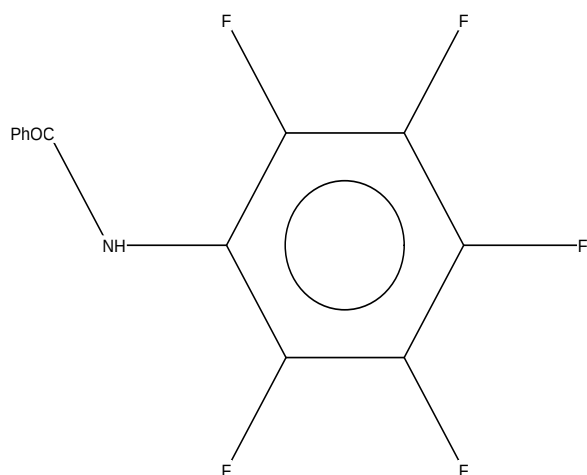
Reference: J.Sopkova, D.S.Hafeed, J.Hodacova, J.Hasek (2000)
Private Communication,

Formula: C₁₃ H₆ F₅ N₁ O₁

Compound Name: 2',3',4',5',6'-Pentafluorobenzoylanilide

Space Group: P2₁/c **Cell:** *a* 4.982(1) *b* 9.724(3) *c* 25.775(9)
Space Group No.: 14 **Cell:** (Å,°) *α* 90.00 *β* 108.43(3) *γ* 90.00(2)

R-Factor (%): 7.17 **Temperature(K)**: 295 **Density(g/cm³)**: 1.610



QUKVUN01

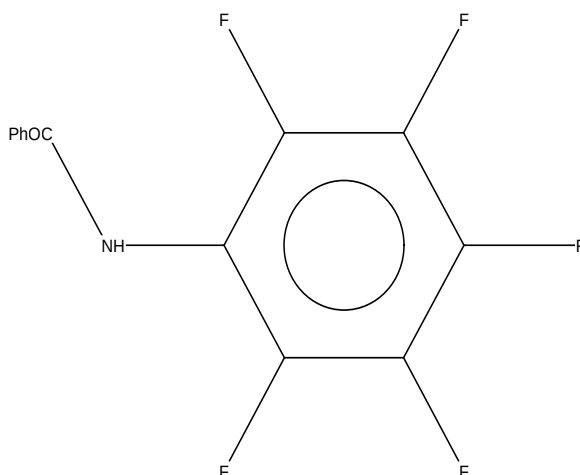
Reference: H.Adams, J.-L.J.Blanco, G.Chessari, C.A.Hunter,
C.M.R.Low, J.M.Sanderson, J.G.Vinter (2001) *Chem.-Eur.J.*, **7**,3494

Formula: C₁₃ H₆ F₅ N₁ O₁

Compound Name: N-Pentafluorophenylbenzamide

Space Group: P-1 **Cell:** *a* 4.831(1) *b* 9.826(5) *c* 24.501(10)
Space Group No.: 2 **Cell:** (Å,°) *α* 89.98(3) *β* 84.98(4) *γ* 89.11(3)

R-Factor (%): 7.49 **Temperature(K)**: 150 **Density(g/cm³)**: 1.647



SAMCAL

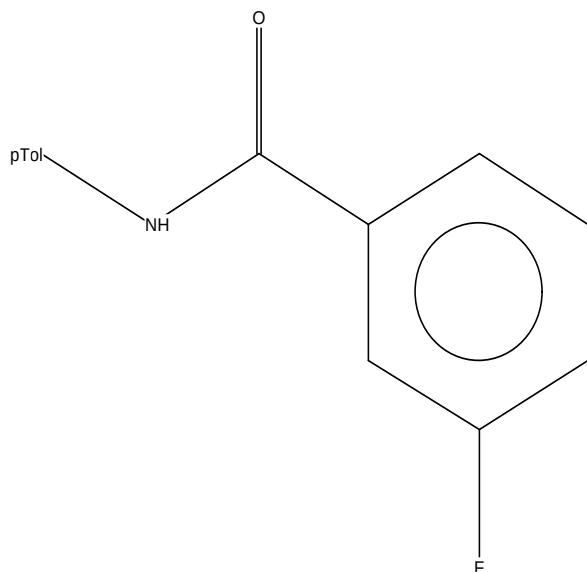
Reference: D.Chopra, T.N.G.Row (2005) *J.Mol.Struct.*, **733**,133

Formula: C₁₄ H₁₂ F₁ N₁ O₁

Compound Name: 3-Fluoro-N-(4-methylphenyl)benzamide

Space Group: P2₁/c **Cell:** *a* 27.388(4) *b* 5.337(0) *c* 7.976(1)
Space Group No.: 14 **Cell:** (Å,°) *α* 90.00 *β* 96.23(0) *γ* 90.00

R-Factor (%): 6.54 **Temperature(K)**: 273 **Density(g/cm³)**: 1.314



SAMCAL01

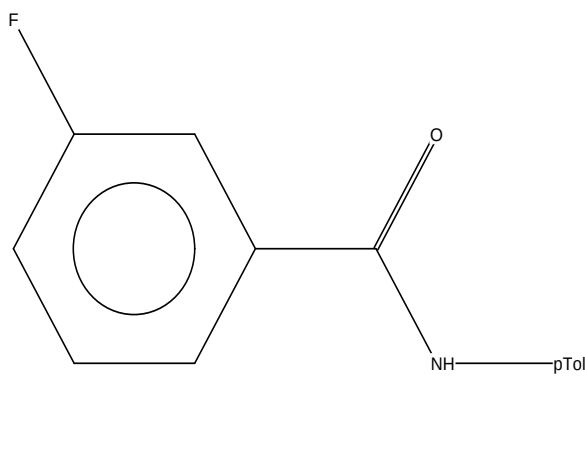
Reference: A.Saeed, R.A.Khera, K.Gotoh, H.Ishida (2008)
Acta Crystallogr., Sect.E:Struct.Rep.Online, **64**,o2098

Formula: C₁₄ H₁₂ F₁ N₁ O₁

Compound Name: 3-Fluoro-N-(p-tolyl)benzamide

Space Group: C2/c **Cell:** *a* 27.645(3) *b* 5.262(0) *c* 15.892(2)
Space Group No.: 15 **Cell:** (Å,°) *α* 90.00 *β* 93.52(0) *γ* 90.00

R-Factor (%): 7.29 **Temperature(K)**: 223 **Density(g/cm³)**: 1.320



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 33-36

TAWRIT

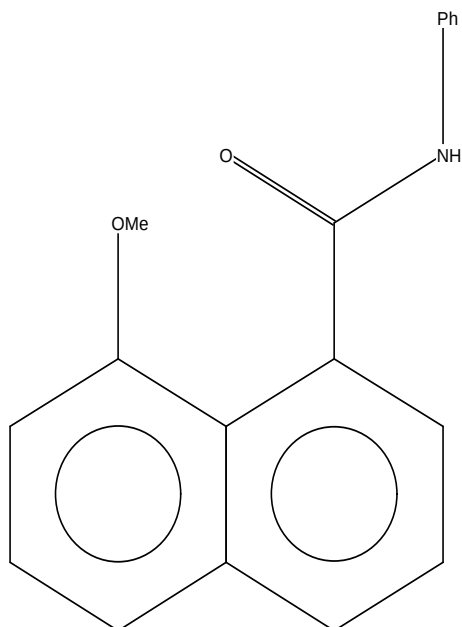
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem. ,3,3273

Formula: C₁₈ H₁₅ N₁ O₂

Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1 **Cell:** *a* 9.771(0) *b* 12.891(0) *c* 13.249(0)
Space Group No.: 2 **Cell:** (*Å*,°) *α* 70.82(0) *β* 68.57(0) *γ* 76.36(0)

R-Factor (%): 6.45 **Temperature(K):** 150 **Density(g/cm³):** 1.266



TAWRIT01

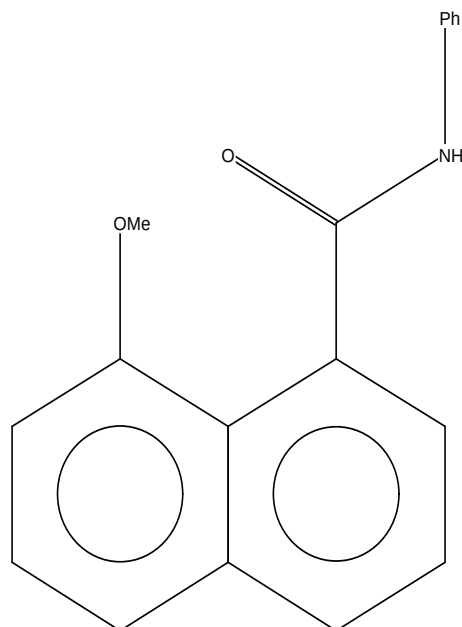
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem. ,3,3273

Formula: C₁₈ H₁₅ N₁ O₂

Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P-1 **Cell:** *a* 10.153(3) *b* 11.463(4) *c* 13.179(7)
Space Group No.: 2 **Cell:** (*Å*,°) *α* 77.35(2) *β* 84.61(4) *γ* 70.15(2)

R-Factor (%): 4.03 **Temperature(K):** 100 **Density(g/cm³):** 1.309



TAWRIT02

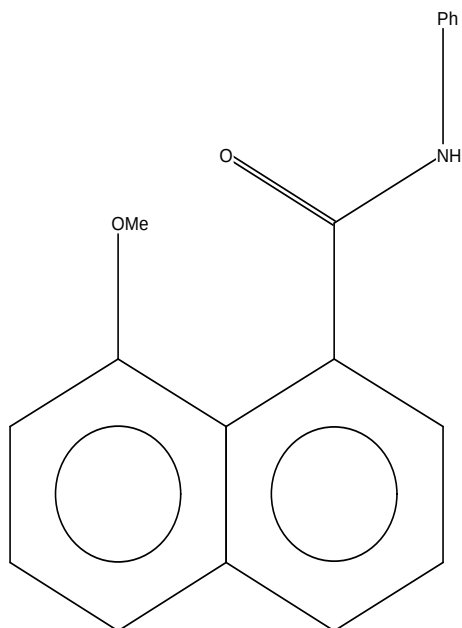
Reference: J.O'Leary, X.Formosa, W.Skranc, J.D.Wallis (2005)
Org.Biomol.Chem. ,3,3273

Formula: C₁₈ H₁₅ N₁ O₂

Compound Name: 8-Methoxy-N-phenyl-1-naphthamide

Space Group: P21/n **Cell:** *a* 10.000(0) *b* 13.128(0) *c* 21.647(0)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 95.70(0) *γ* 90.00

R-Factor (%): 3.70 **Temperature(K):** 100 **Density(g/cm³):** 1.303



WAKCIW

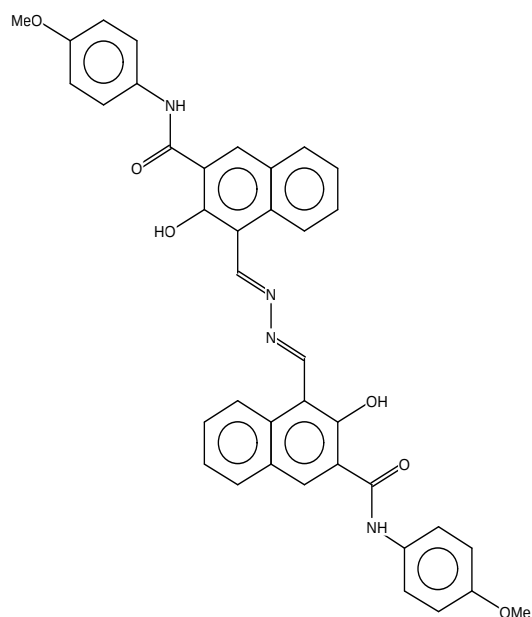
Reference: J.Bruning, E.Alig, A.Meents, J.van de Streek, M.U.Schmidt
(2009) *Z.Kristallogr.* ,224,556

Formula: C₃₈ H₃₀ N₄ O₆

Compound Name: 4,4'-(Hydrazine-1,2-diylidenedimethylidene)-bis(3-hydroxy-N-(4-methoxyphenyl)-2-naphthamide)

Space Group: P21/c **Cell:** *a* 4.917(1) *b* 27.672(6) *c* 11.101(2)
Space Group No.: 14 **Cell:** (*Å*,°) *α* 90.00 *β* 105.05(3) *γ* 90.00

R-Factor (%): 5.78 **Temperature(K):** 100 **Density(g/cm³):** 1.454



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 37-40

WAKCIW01

Reference: J.Bruning, E.Alig, A.Meents, J.van de Streek, M.U.Schmidt (2009) *Z.Kristallogr.* ,**224**,556

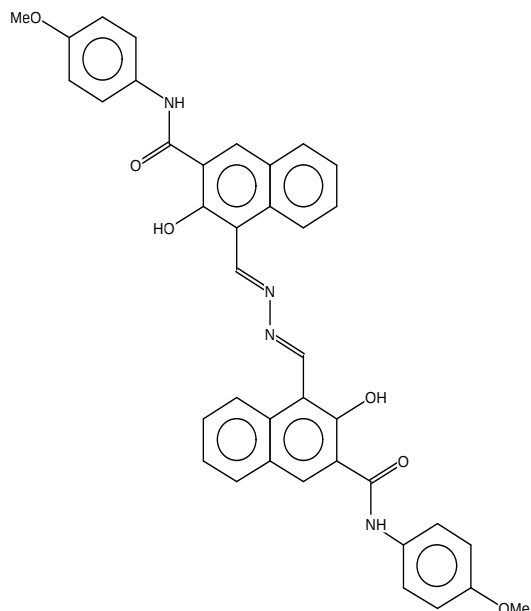
Formula: C₃₈ H₃₀ N₄ O₆

Compound Name: 4,4'-(Hydrazine-1,2-diylidenedimethylidene)-bis(3-hydroxy-N-(4-methoxyphenyl)-2-naphthamide)

Space Group: P2₁/c
Space Group No.: 14
R-Factor (%): 3.48

Cell: **a** 5.180(0) **b** 25.836(1) **c** 12.157(0)
(Å,°) **α** 90.00 **β** 110.69(0) **γ** 90.00

Temperature(K): 293 **Density(g/cm³):** 1.394



XAVTOF

Reference: D.Grillo, G.Polla, D.Vega (2012) *J.Pharm.Sci.* ,**101**,541

Formula: C₂₉ H₃₂ N₇ O₁¹⁺·C₁ H₃ O₃ S₁¹⁻

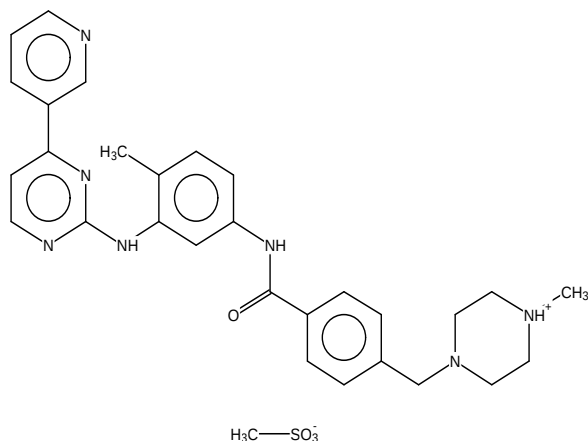
Compound Name: 1-Methyl-4-{4-((4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)carbamoyl)benzyl}piperazin-1-ium methanesulfonate

Synonym: Imatinib mesylate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.24

Cell: **a** 9.336(0) **b** 9.862(0) **c** 18.024(0)
(Å,°) **α** 81.30(0) **β** 90.02(0) **γ** 63.11(0)

Temperature(K): 150 **Density(g/cm³):** 1.343



XAVTOF01

Reference: D.Grillo, G.Polla, D.Vega (2012) *J.Pharm.Sci.* ,**101**,541

Formula: C₂₉ H₃₂ N₇ O₁¹⁺·C₁ H₃ O₃ S₁¹⁻

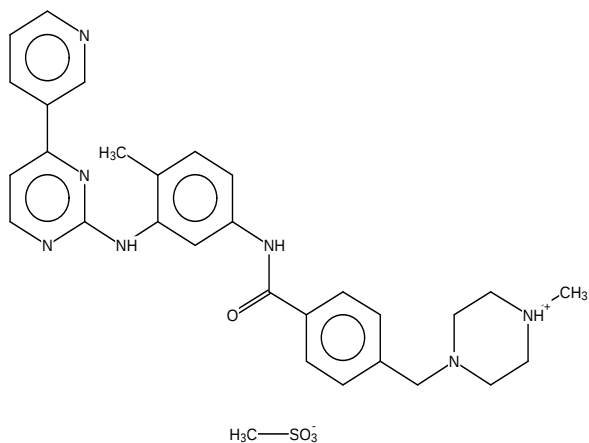
Compound Name: 1-Methyl-4-{4-((4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)carbamoyl)benzyl}piperazin-1-ium methanesulfonate

Synonym: Imatinib mesylate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 5.92

Cell: **a** 9.479(0) **b** 9.881(0) **c** 18.099(1)
(Å,°) **α** 80.95(0) **β** 89.41(0) **γ** 62.62(0)

Temperature(K): 293 **Density(g/cm³):** 1.321



XAVTOF02

Reference: D.Grillo, G.Polla, D.Vega (2012) *J.Pharm.Sci.* ,**101**,541

Formula: C₂₉ H₃₂ N₇ O₁¹⁺·C₁ H₃ O₃ S₁¹⁻

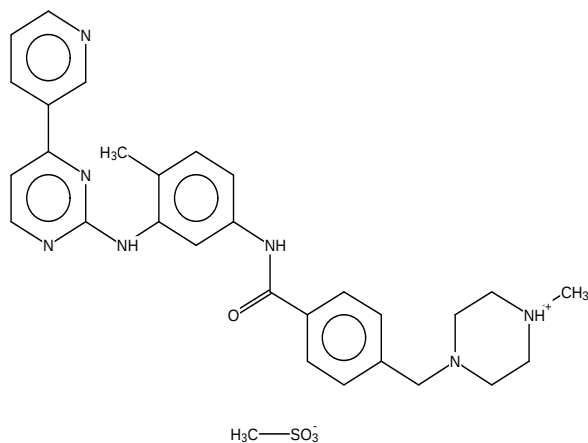
Compound Name: 1-Methyl-4-{4-((4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)carbamoyl)benzyl}piperazin-1-ium methanesulfonate

Synonym: Imatinib mesylate

Space Group: P-1
Space Group No.: 2
R-Factor (%): 3.34

Cell: **a** 9.109(0) **b** 10.464(0) **c** 15.070(0)
(Å,°) **α** 93.46(0) **β** 93.61(0) **γ** 90.39(0)

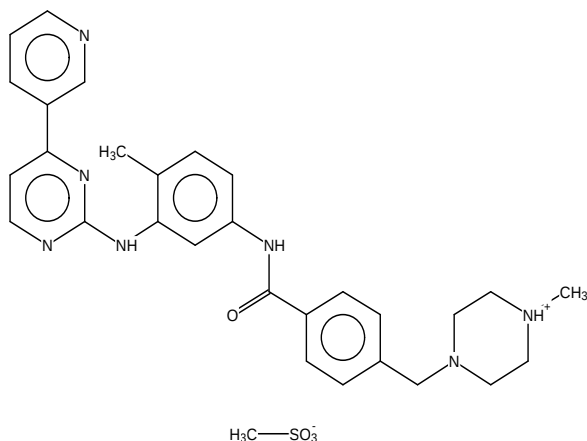
Temperature(K): 150 **Density(g/cm³):** 1.369



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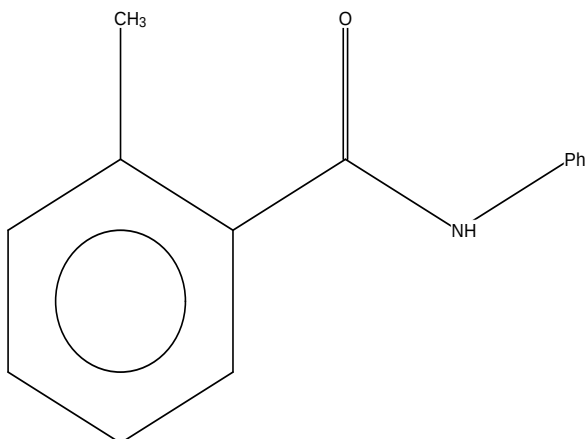
XAVTOF03

Reference: D.Grillo, G.Polla, D.Vega (2012) *J.Pharm.Sci.* ,**101**,541
Formula: $C_{29}H_{32}N_7O_1^{1+}, C_1H_3O_3S_1^{1-}$
Compound Name: 1-Methyl-4-(4-((4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)carbamoyl)benzyl)piperazin-1-ium methanesulfonate
Synonym: Imatinib mesylate
Space Group: P-1
Space Group No.: 2
R-Factor (%): 4.12
Cell: a 9.113(0) b 10.523(0) c 15.260(1)
 α 93.36(0) β 93.82(0) γ 90.81(0)
Temperature(K): 293 **Density(g/cm³):** 1.344



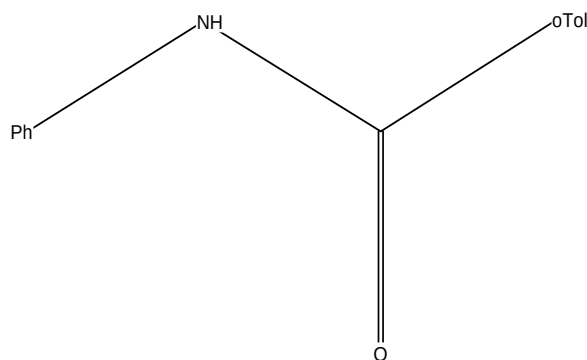
YEGJID

Reference: I.Azumaya, K.Yamaguchi, H.Kagechika, S.Saito, A.Itai, K.Shudo (1994) *Yakugaku Zasshi(Jap.)(J.Pharm.Soc.Jpn.)* ,**114**,414
Formula: $C_{14}H_{13}N_1O_1$
Compound Name: trans-2-Methylbenzanilide
Space Group: P21/c
Space Group No.: 14
R-Factor (%): 5.20
Cell: a 5.067(1) b 19.429(1) c 11.506(1)
 α 90.00 β 92.27(1) γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.240



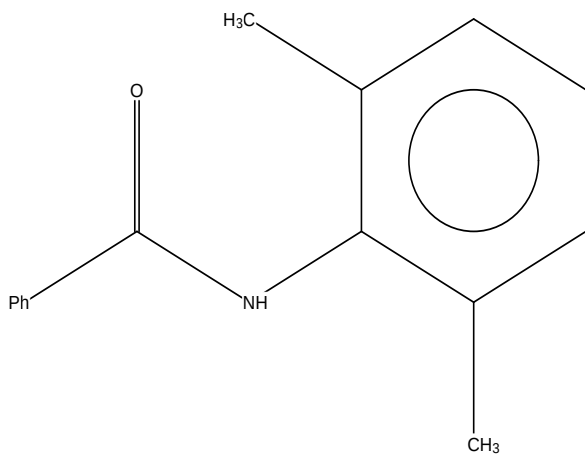
YEGJID01

Reference: B.T.Gowda, S.Foro, B.P.Sowmya, H.Fuess (2008) *Acta Crystallogr., Sect.E: Struct. Rep. Online* ,**64**,o383
Formula: $C_{14}H_{13}N_1O_1$
Compound Name: 2-Methyl-N-phenylbenzamide
Space Group: Pbca
Space Group No.: 61
R-Factor (%): 3.78
Cell: a 14.404(1) b 8.682(0) c 18.710(1)
 α 90.00 β 90.00 γ 90.00
Temperature(K): 100 **Density(g/cm³):** 1.199



YEGJUP

Reference: I.Azumaya, K.Yamaguchi, H.Kagechika, S.Saito, A.Itai, K.Shudo (1994) *Yakugaku Zasshi(Jap.)(J.Pharm.Soc.Jpn.)* ,**114**,414
Formula: $C_{15}H_{15}N_1O_1$
Compound Name: trans-2',6'-Dimethylbenzanilide
Space Group: Pbca
Space Group No.: 61
R-Factor (%): 5.90
Cell: a 9.602(6) b 31.381(8) c 8.329(1)
 α 90.00 β 90.00 γ 90.00
Temperature(K): 295 **Density(g/cm³):** 1.193



Search: search1 (Sun Feb 03 13:27:04 2013): Hits 45-48

YEGJUP01

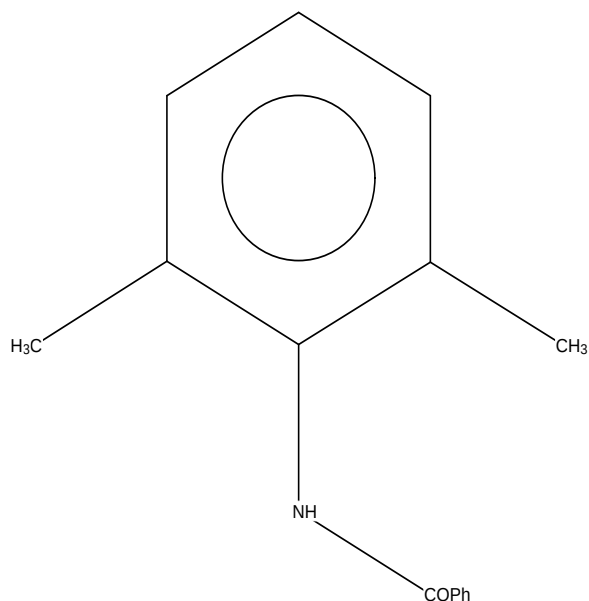
Reference: B.T.Gowda, M.Tokarcik, J.Kozisek, B.P.Sowmya, H.Fuess (2008) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**64**,o1299

Formula: C₁₅ H₁₅ N₁ O₁

Compound Name: N-(2,6-Dimethylphenyl)benzamide

Space Group: Pc **Cell:** **a** 16.439(0) **b** 8.290(0) **c** 9.490(0)
Space Group No.: 7 **Cell:** **(Å,°)** **α** 90.00 **β** 98.17(0) **γ** 90.00

R-Factor (%): 3.90 **Temperature(K)**: 295 **Density(g/cm³)**: 1.169



YODFAZ

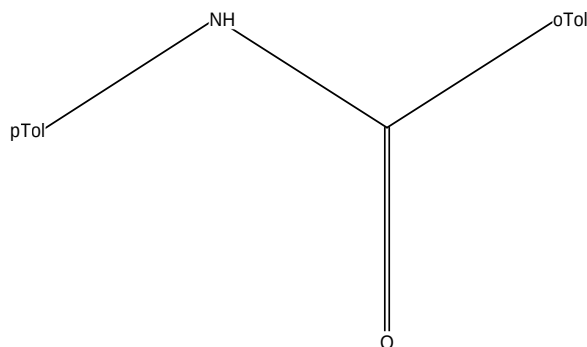
Reference: B.T.Gowda, M.Tokarcik, J.Kozisek, B.P.Sowmya, H.Fuess (2008) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**64**,o1494

Formula: C₁₅ H₁₅ N₁ O₁

Compound Name: 2-Methyl-N-(4-methylphenyl)benzamide

Space Group: C2/c **Cell:** **a** 40.663(1) **b** 7.177(0) **c** 8.942(0)
Space Group No.: 15 **Cell:** **(Å,°)** **α** 90.00 **β** 96.17(0) **γ** 90.00

R-Factor (%): 4.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.154



YODFAZ01

Reference: A.Saeed, R.A.Khera, J.Simpson (2010) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**66**,o911

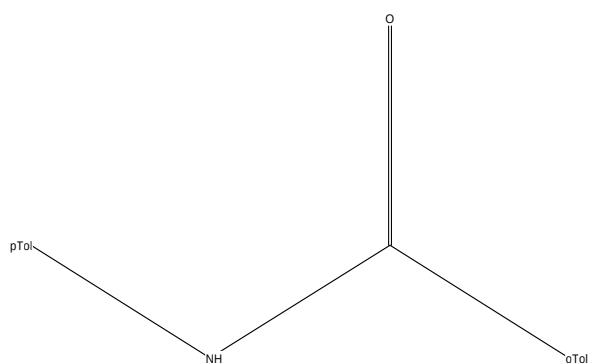
Formula: C₁₅ H₁₅ N₁ O₁

Compound Name: 2-Methyl-N-(4-methylphenyl)benzamide

Synonym: 2-methyl-N-p-tolylbenzamide

Space Group: P21/c **Cell:** **a** 20.259(3) **b** 7.068(1) **c** 8.794(1)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 95.94(0) **γ** 90.00

R-Factor (%): 3.99 **Temperature(K)**: 89 **Density(g/cm³)**: 1.195



YOTROP

Reference: A.Saeed, M.Irfan, M.Bolte (2009) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**65**,o1334

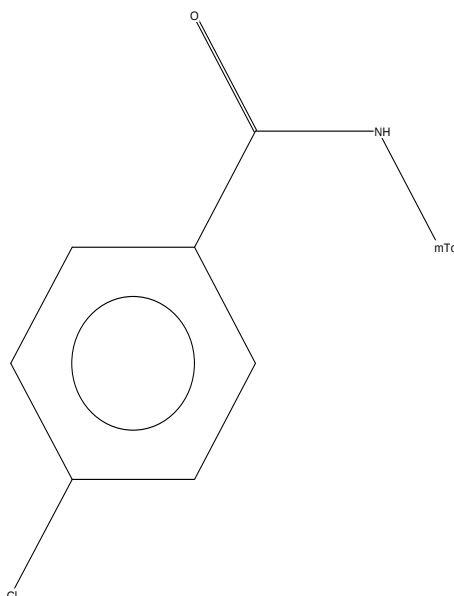
Formula: C₁₄ H₁₂ Cl₁ N₁ O₁

Compound Name: 4-Chloro-N-(3-methylphenyl)benzamide

Synonym: 4-Chloro-N-m-tolylbenzamide

Space Group: P21/c **Cell:** **a** 13.972(1) **b** 10.192(0) **c** 9.015(0)
Space Group No.: 14 **Cell:** **(Å,°)** **α** 90.00 **β** 105.42(0) **γ** 90.00

R-Factor (%): 6.60 **Temperature(K)**: 173 **Density(g/cm³)**: 1.319



Search: search1 (Sun Feb 03 13:27:04 2013): Hit 49

YOTROP01

Reference: V.Z.Rodrigues, M.Fronc, B.T.Gowda, J.Kozisek (2011)
Acta Crystallogr., Sect.E: Struct. Rep. Online ,67,o2903

Formula: C₁₄ H₁₂ Cl₁ N₁ O₁

Compound Name: 4-Chloro-N-(3-methylphenyl)benzamide

Space Group: P2₁/c **Cell:** **a** 13.438(0) **b** 10.249(1) **c** 9.260(0)
Space Group No.: 14 (**Å, °**) **α** 90.00 **β** 92.89(0) **γ** 90.00
R-Factor (%): 4.03 **Temperature(K)**: 293 **Density(g/cm³)**: 1.281

