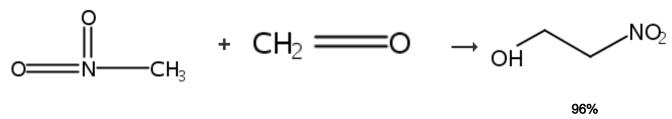
1. Single Step



Overview

Steps/Stages

1.1 R:K₂CO₃, S:EtOH, 3 h, reflux

Notes

paraformaldehyde used, reactant also recovered as product, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Process for preparation of taurine and bicarbonate

By Sun, Huajun et al

From Faming Zhuanli Shenqing, 105693559, 22 Jun 2016

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2. Single Step

$$0 = N - CH_3 + CH_2 = 0 \rightarrow OH - NO_2$$

Overview

Steps/Stages

1.1 R:KOH, S:MeNO₂, S:H₂O, 2 h, rt; 30 min, 100° C; 100° C \rightarrow rt

Notes

Reactants: 2, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Organocatalytic Enantioselective Formal C(sp2)-H Alkylation

By Manna, Madhu Sudan and Mukherjee, Santanu

From Journal of the American Chemical Society, 137(1), 130-133; 2015

Experimental Procedure

Preparation of 2-nitroethan-1-ol (2j): In an oven-dried round-bottom flask, equipped with reflux condenser, paraformaldehyde (500 mg, 16.65 mmol, 1.0 equiv.) was taken with 75.0 mL of nitromethane. To this was added 0.15 mL 3.0 M methanolic KOH solution and the mixture was stirred at r.t. for 2 h and then refluxed at 100 °C for additional 30 min. After cooling the reaction mixture to r.t., solvent was removed under reduced pressure and the residue was purified by silica-gel column chromatography (20-25% EtOAc in petroleum ether). 2j as a light yellow oil (910 mg, 1.00 mmol, 60% yield). FT-IR (Thin film): 2921 (w), 1637 (m), 1402 (w), 1261 (m); 1H-NMR (400 MHz, CDCl₃): δ 4.51 (t, J = 4.7 Hz, 2H), 4.12-4.10 (m, 2H), 2.93 (br s, 1H); 13 C-NMR (100 MHz, CDCl₃): δ 77.2, 58.7.

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3. Single Step

$$0 \longrightarrow N \longrightarrow CH_3 + CH_2 \longrightarrow OH \longrightarrow OH \longrightarrow NO_2$$

Overview

Steps/Stages

1.1 R:NaOH, S:MeOH, 5 h, rt; 2 h, reflux

Notes

paraformaldehyde used, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

A process for preparing taurine

By Sun, Huajun et al From Faming Zhuanli Shenqing, 103613517, 05 Mar 2014

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4. Single Step

$$O = N - CH_3 + CH_2 = O \rightarrow OH - NO_2$$

Overview

Steps/Stages

1.1 R:KOH, S:MeOH

Notes

Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Asymmetric synthesis of aphanorphine and synthetic approaches towards dietyoxetane

By Welsh, Emma Jane From null, , No pp.; 2007

Experimental Procedure

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The crude nitroethanol 533 (518 was author's error): A three necked round bottomed flask was equipped with a dropping funnel, thermometer and a condenser. Paraformaldehyde (18.0 g, 0.6 mol) and freshly distilled nitromethane (340 mL, 6.7 mol) were added to the flask and the mixture was stirred vigorously. KOH (3 M in MeOH, Ca. 1.5 mL) was added dropwise through the dropping funnel until pH 8 was reached (litmus paper). The mixture became homogenous after 20 min and the solution was stirred at rt for 1 hr. Conc. H2SO4 was added until the solution reached pH 4 and the solution was stirred at rt overnight. The reaction mixture was subjected to vacuum filtration and the filtrate (66 g) was added to a flask containing diphenyl ether (66 g). The solution was distilled under reduced pressure (0.8 mbar). The first fraction to distil contained unreacted nitromethane (bp 24 degC), the second fraction contained nitroethanol and diphenyl ether (bp 84 degC). The second fraction was biphasic and the lower layer was removed and washed with hexane (30 mL). The lower layer was separated to afford nitroethanol (23.88 g, 44 %) and was used without further purification.

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5. Single Step

$$O = N - CH_3 + CH_2 = O \rightarrow OH - NO_2$$

Overview

Steps/Stages

1.1 S:H₂O

Notes

Reactants: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Studies towards the total synthesis of (-)mitragynine using solid-supported reagents

By Henry, D. J.

From null, , No pp.; 2003

Experimental Procedure

2-Nitroethanol 90: Formaldehyde (67 % aqueous solution) (10 mL, 193 mmol) was added to a suspension of polymer-supported hydroxide (95 g, 285 mmol) in nitromethane (200 mL) and the reaction mixture stirred at rt for 10 min. The mixture was filtered, the beads washed extensively with nitromethane (3 x 100 mL) and CH2Cl2 (5 x 100 mL) and the solvent then removed in vacuo. The resultant yellow oil was redissolved in CH2Cl2 (100 mL), dried (MgSO4) and the solvent removed in vacuo to afford 2-nitroethanol 90 as a yellow oil (3.96 g, 23 %).

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6. Single Step

$$CH_2 \longrightarrow CH_2 \rightarrow OH \longrightarrow NO_2 + O_2 N \longrightarrow NO_2$$

Overview

1.1

Go to Science of Synthesis, a critically reviewed reference work of synthetic methodology, for more information., Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Product class 1: Synthesis of nitroalkanes

By Aitken, R. A. and Aitken, K. M. From Science of Synthesis, 41, 9-258; 2010

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7. Single Step

Overview

Steps/Stages

1.1

Notes

Go to Science of Synthesis, a critically reviewed reference work of synthetic methodology, for more information., Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Product class 1: Synthesis of nitroalkanes

By Aitken, R. A. and Aitken, K. M. From Science of Synthesis, 41, 9-258; 2010

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8. Single Step

$$CH_2 \longrightarrow CH_2 \longrightarrow OH \longrightarrow NO_2 + O_2 N \longrightarrow$$

Overview

1.1

Go to Science of Synthesis, a critically reviewed reference work of synthetic methodology, for more information., Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Product class 1: Synthesis of nitroalkanes

By Aitken, R. A. and Aitken, K. M. From Science of Synthesis, 41, 9-258; 2010

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9. Single Step



Overview

Steps/Stages

1.1

Notes

Go to Science of Synthesis, a critically reviewed reference work of synthetic methodology, for more information., Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Product class 1: Synthesis of nitroalkanes

By Aitken, R. A. and Aitken, K. M.

From Science of Synthesis, 41, 9-258; 2010

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10. Single Step

$$0 \longrightarrow N \longrightarrow CH_3 + CH_2 \longrightarrow O \longrightarrow OH \longrightarrow NO_2$$

Overview

1.1 R:NaF, S:Me₂CHOH, 20 h, 40°C

paraformaldehyde used, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Method for synthesis of Florfenicol intermediate (1R,2R)-2-amino-1-(4-(methylsulphonyl)phenyl)-1,3-propanediol

By Peng, Yaowu et al

From Faming Zhuanli Shenqing, 101941927, 12 Jan 2011

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11. Single Step

$$Br$$
 + CH_2 O O O

Overview

Steps/Stages

- 1.1 R:In, S:THF, 20 min
- 1.2 S:H₂O, 4 h
- 1.3 R:NaHCO₃, S:H₂O

Notes

ultrasound, regioselective, paraformaldehyde used, Reformatsky reaction, Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stages: 3, Most stages in any one step: 3

References

Convenient procedure for the indiummediated hydroxymethylation of active bromo compounds: transformation of ketones into α -hydroxymethyl nitroalkanes

By Soengas, Raquel G. and Estevez, Amalia M.

From Synlett, (17), 2625-2627; 2010

Experimental Procedure

General Procedure for the hydroxymethylation of 2-bromonitroalkanes: To a suspension of indium powder (0.5 mmol) in THF (1 mL), bromonitroalkane (0.75 mmol) was added and the mixture was sonicated for 20 min. Paraformaldehyde (0.5 mmol) was then added and sonication continued for further 4 h. The reaction mixture was neutralized with saturated aqueous sodium hydrogen carbonate, diluted with water (10 mL) and extracted with ether (3 x 25 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was evaporated in vacuo to obtain pure compounds shown in Table 4. Nitroethanol, clear oil, yield 31.3 mg, 69%. ¹H-NMR (CDCl₃, ppm): 3.72-3.76 (m, 2H); 4.18-4.34 (m, 2H). ¹³C NMR (CDCl₃, ppm): 59.8 (C-1); 78.5 (C-2).

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12. Single Step

$$0 = N - CH_3 + CH_2 = O \rightarrow OH$$
 38%

Overview

Steps/Stages

1.1 C:PhCH₂N+Me₃ •OH-, S:H₂O, S:MeOH, 66 h, rt

Notes

Henry reaction, Reactants: 2, Catalysts: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Solvent effect on the reversibility of base catalyzed Henry reactions - Triton B catalyzed nitro aldol reactions in alcohol

By Ono, Fumiyasu et al

From Sogo Rikogaku Hokoku (Kyushu Daigaku Daigakuin), 30(1), 25-28; 2008

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13. Single Step

Overview

Steps/Stages

1.1 R:CeCl₃, R:Nal, S:MeCN, 32 h, 70°C

Notes

chemoselective, optimization study, Reactants: 1, Reagents: 2, Solvents: 1, Steps: 1, Stages:

1, Most stages in any one step: 1

References

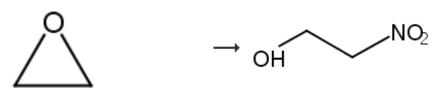
tert-Butyl ethers: renaissance of an alcohol protecting group. Facile cleavage with Cerium(III) chloride/sodium iodide

By Bartoli, Giuseppe et al

From Advanced Synthesis & Catalysis, 348(7+8), 905-910; 2006

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14. Single Step



Overview

Steps/Stages

1.1 R:NaNO₂, C:10025-84-0, C:Bu₄N+ •Br-, S:H₂O, S:Et₂O, 6 h, -5°C

Notes

Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

LaCl3.7H2O-promoted regioselective ring opening of epoxides using NaNO2 in etherwater system. A facile synthesis of 2-nitroalcohols

By Borah, Jagat C. et al

From Synthetic Communications, 35(6), 873-878; 2005

Experimental Procedure

General Procedure for the Ring Opening of Epoxides A mixture of the epoxide (3.05 mmol), NaNO₂ (1.68 g, 24.4 mmol), LaCl₃.bul.7H₂O (2.27 g, 6.11 mmol), and Bu₄NBr (0.2 g, 0.62 mmol) in ether: water (1:1) system was vigorously stirred at room temperature. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was extracted with ether, dried over anhydrous Na₂SO₄ and concentrated. The crude product was purified by preparative TLC using 1:5 ethyl acetate: hexane. *Table 1*, Entry 1, yield 78%.

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15. Single Step

$$CH_2 \longrightarrow O + O \longrightarrow N \longrightarrow O \longrightarrow OH \longrightarrow NO_2$$

Overview

Steps/Stages

1.1

Notes

Reactants: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Nitroethylene: a stable, clean, and reactive agent for organic synthesis

By Ranganathan, Darshan et al From Journal of Organic Chemistry, 45(7), 1185-9; 1980

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16. Single Step

$$0 \longrightarrow N \longrightarrow CH_3 + CH_2 \longrightarrow OH \longrightarrow OH \longrightarrow NO_2$$

49%

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Overview

Steps/Stages

1.1 R:KOH, S:H₂O, S:MeNO₂

Notes

Paraformaldehyde, KOH/MeOH, MeNO2, r.t./1 h., Hydroxymethylation, Reactants: 2, Reagents: 1, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

2-Nitroethanol

By Noland, Wayland E.

From Organic Syntheses, 41, 67-72; 1961

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17. Single Step

$$0 \longrightarrow N \longrightarrow CH_3 + CH_2 \longrightarrow O \longrightarrow OH \longrightarrow NO_2$$

Overview

Steps/Stages

1.1 R:K₂CO₃, S:H₂O

Notes

Classification: C-Alkylation; # Conditions: K2CO3 H2O; 3h Rf, Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Nitroethylene

By Hopff, H. and Capaul, M. From Helvetica Chimica Acta, 43, 1898-910; 1960

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18. Single Step

Overview

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1.1 R:AgNO₂, S:Et₂O

Classification: Substitution; C-Nitration; # Conditions: AgNO2 Et2O; Rf 3h, Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

The nitroethylation of indole. A new synthesis of tryptamine

By Noland, Wayland E. and Hartman, Philip J. From Journal of the American Chemical Society, 76, 3227-8; 1954

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