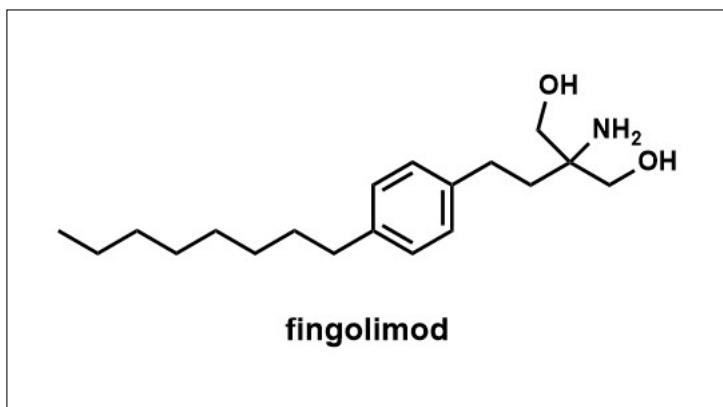


Fingolimod



Related reviews in Science of Synthesis

- β -Amino Alcohols
- 1,3-Diols
- Alkylarenes
- Friedel–Crafts Acylation
- Reduction of Aryl Alkyl Ketones Using Organosilanes
- Kumada Cross-Coupling Reactions

Synonyms: FTY-720

ATC: L04AA27

Use: Immunomodulator

Chemical name: 2-Amino-2-[2-(4-octylphenyl)ethyl]-1,3-propanediol

Formula: $C_{19}H_{33}NO_2$

MW: 307.48 g/mol

CAS-RN: 162359-55-9

InChI Key: KKGQTZUTZRNORY-UHFFFAOYSA-N

InChI: InChI=1S/C19H33NO2/c1-2-3-4-5-6-7-8-17-9-11-18(12-10-17)13-14-19(20,15-21)16-22/h9-12,21-22H,2-8,13-16,20H2,1H3

Derivatives

hydrochloride

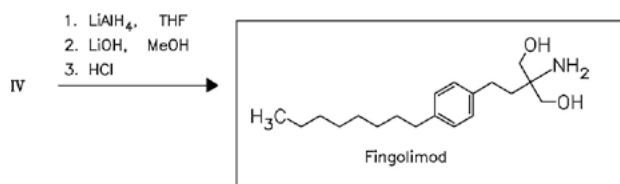
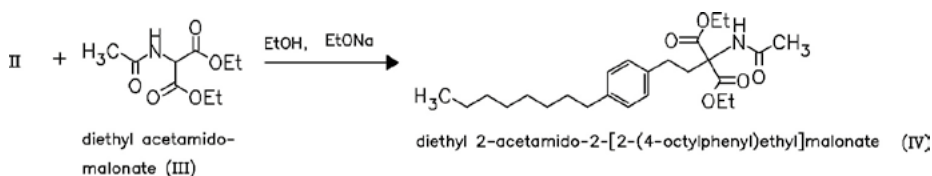
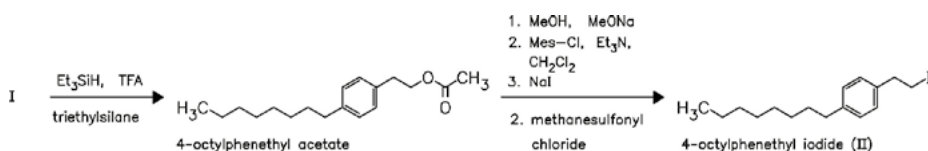
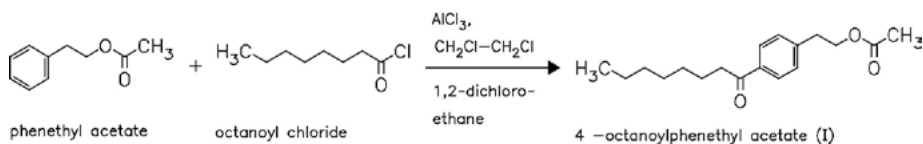
Formula: $C_{19}H_{33}NO_2 \cdot HCl$

MW: 343.94 g/mol

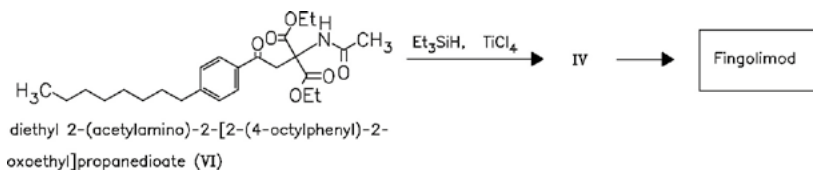
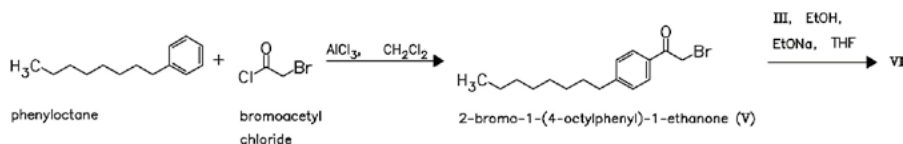
CAS-RN: 162359-56-0

Synthesis Path

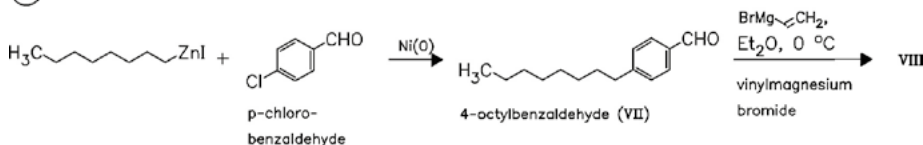
a)

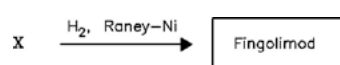
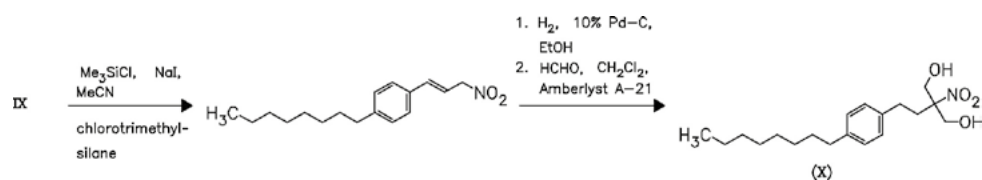
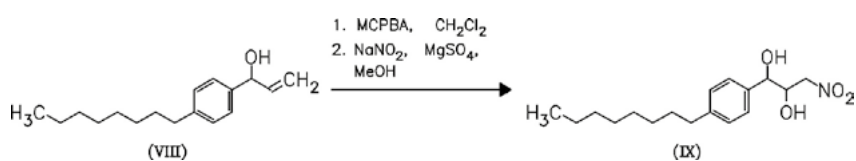


b)

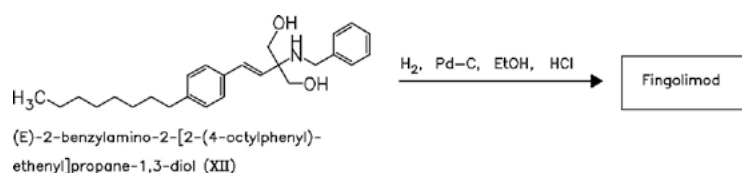
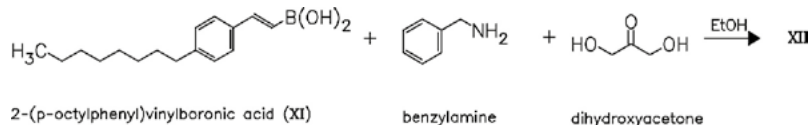
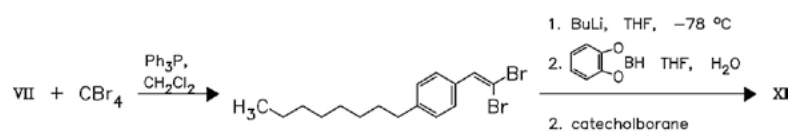


c)

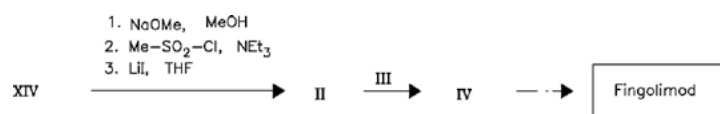
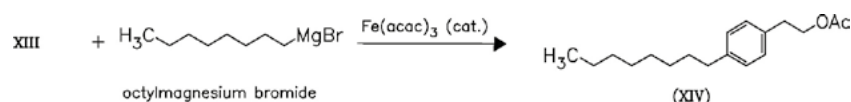
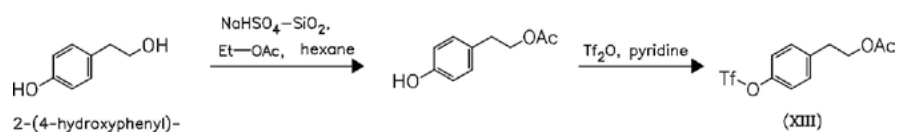




d



e



Substances Referenced in Synthesis Path

| CAS-RN | Formula | Chemical Name | CAS Index Name |
|-------------|---|---|--|
| | C ₁₁ H ₁₁ F ₃ O ₅ S | 4-[2-(acetyloxy)ethyl]phenyl trifluoromethanesulfonate | |
| 100-46-9 | C ₇ H ₉ N | benzylamine | Benzenemethanamine |
| | C ₂₆ H ₃₉ NO ₂ | (E)-2-benzylamino-2-[2-(4-octylphenyl)ethenyl]-propane-1,3-diol | |
| 22118-09-8 | C ₂ H ₂ BrClO | bromoacetyl chloride | Acetyl chloride, bromo- |
| | C ₁₆ H ₂₃ BrO | 2-bromo-1-(4-octylphenyl)-1-ethanone | |
| 104-88-1 | C ₇ H ₅ ClO | 4-chlorobenzaldehyde | Benzaldehyde, 4-chloro- |
| | C ₁₆ H ₂₂ Br ₂ | 2-(2,2-dibromoethenyl)-4-octylbenzene | |
| 1068-90-2 | C ₉ H ₁₅ NO ₅ | diethyl acetamidomalonate | Propanedioic acid, (acetylamino)-, diethyl ester |
| | C ₂₅ H ₃₉ NO ₅ | diethyl (acetylamino)[2-(4-octylphenyl)ethyl]malonate | |
| | C ₂₄ H ₃₇ NO ₆ | diethyl 2-(acetylamino)-2-[4-(octylphenyl)-2-oxoethyl]propanedioate | |
| 96-26-4 | C ₃ H ₆ O ₃ | 1,3-dihydroxyacetone | 2-Propanone, 1,3-dihydroxy- |
| | C ₁₇ H ₂₆ O | α-ethenyl-4-octylbenzenemethanol | |
| 141-78-6 | C ₄ H ₈ O ₂ | ethyl acetate | Acetic acid ethyl ester |
| 50-00-0 | CH ₂ O | formaldehyde | Formaldehyde |
| 58556-55-1 | C ₁₀ H ₁₂ O ₃ | 4-hydroxbenzenethanol α-acetate | |
| 501-94-0 | C ₈ H ₁₀ O ₂ | 2-(4-hydroxyphenyl)ethanol | |
| 374077-88-0 | C ₁₉ H ₃₁ NO ₄ | 2-nitro-2-[2-(4-octylphenyl)ethyl]-1,3-propanediol | |
| 374077-82-4 | C ₁₇ H ₂₇ NO ₄ | 3-nitro-1-(4-octylphenyl)-1,2-propanediol | |
| 374077-86-8 | C ₁₇ H ₂₅ NO ₂ | 1-(3-nitro-1-propenyl)-4-octylbenzene | |
| 111-64-8 | C ₈ H ₁₅ ClO | octanoyl chloride | Octanoyl chloride |
| | C ₁₈ H ₂₆ O ₃ | 4-octanoylphenethyl acetate | |
| 49763-66-8 | C ₁₅ H ₂₂ O | 4-octylbenzaldehyde | |
| | C ₁₈ H ₂₈ O ₂ | 4-octylbenzeneethanol acetate | |
| 17049-49-9 | C ₈ H ₁₇ BrMg | octylmagnesium bromide | |
| | C ₁₈ H ₂₈ O ₂ | 4-octylphenethyl acetate | |
| | C ₁₆ H ₂₅ I | 4-octylphenethyl iodide | |
| | C ₁₆ H ₂₅ BO ₂ | [2-(4-octylphenyl)ethenyl]boronic acid | |
| | C ₈ H ₁₇ I ₂ Zn | octylzinc iodide | |
| 103-45-7 | C ₁₀ H ₁₂ O ₂ | phenethyl acetate | |
| 2189-60-8 | C ₁₄ H ₂₂ | phenylcatane | |
| 558-13-4 | CBr ₄ | tetrabromomethane | |
| 3536-96-7 | C ₂ H ₃ ClMg | vinylmagnesium chloride | Magnesium, chloroethenyl- |

Trade Names

| Country | Trade Name | Vendor |
|---------|------------|----------------|
| USA | Gilenia | Novartis, 2010 |

Formulations

cps. 0,5 mg

References

- Adachi, K. et al.: Bioorg. Med. Chem. Lett. (BMCLE8) **5**, 847 (1995).
 Adachi, K. et al.: Bioorg. Med. Chem. Lett. (BMCLE8) **5**, 853 (1995).
 Kiuchi, M. et al.: J. Med. Chem. (JMCMAR) **43**, 2946-2961 (2000).
b Durand, P. et al.: Synthesis (SYNTBF) **4**, 505-506 (2000).
c Kalita, B. et al.: Synlett (SYNLES) **9**, 1411-1414 (2001).
d Sugiyama, S. et al.: Chem. Pharm. Bull. (CPBTAL) **53**, 100-102 (2005).
e Seidel, G. et al.: J. Org. Chem. (JOCEAH) **69**, 3950-3952 (2004).
a EP 0 627 406 (Yoshitomi Pharm.; 28.4.1994; appl. 18.10.1993; J-prior. 21.10.1992).
for chiral analogues see:
 Hinterding, K. et al.: Tetrahedron Lett. (TELEAY) **43**, 8095-8097 (2002).
 Zhu, R. et al.: J. Med. Chem. (JMCMAR) **50**, 6428-6435 (2007).
use of 1,3-propanediol derivatives:
 US 6 486 209 (Novartis AG; 26.11.2002; appl. 3.7.2001; GB-prior. 19.11.1996).