

[🏠](#) / substances / ZINC000013520815

# ZINC13520815 (Alora)

[Google](#) [Wikipedia](#) [PubMed](#)

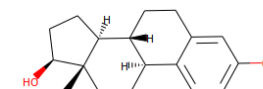
Added	Availability	Since	Mwt	logP	Download
2008-06-21	In-Stock	2015-08-07	272.388	3.609	<a href="#">↓</a>

Mol Formula	Rings	Heavy Atoms	Hetero Atoms	Fraction sp <sup>3</sup>	Tranche
C18H24O2	4	20	2	0.67	CHAA

SMILES	<chem>C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@H]2</chem>	<a href="#">📄</a>
InChI	InChI=1S/C18H24O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(	<a href="#">📄</a>
InChI Key	VOXZDWNPVJITMN-ZBRFXRBCSA-N	<a href="#">📄</a>

## Available 3D Representations





pH range	Net charge	H-bond donors	H-bond acceptors	tPSA	Rotatable bonds	Apolar desolvation	Polar desolvation	Download
						n	n	
Reference	0	2	2	40	0	4.82	-5.17	<a href="#">↓</a>










Draw

96 Items Total

87 Items Total






Vendors (64 Total)		
Cayman Chemical		10006315
MedChem Express		HY-B0141
Economical		
TargetMol Bioactives		T1048
Tocris		2824
Combi-Blocks		JW-2193
Sigma Aldrich		1250008, 31734, 3301, BP729, E-060, E1024, E1132, E1620000, E2257, E2758, E8875, PHR1353
(Building Blocks)		
Accela ChemBio Inc		SY017569
AK Scientific		H061, J10189
Economical		
APExBIO		A8425
Rosche Scientific		E0342

Annotated Catalogs (57 Total)		
Illuminating the		NCC-1-1-B-9,
Druggable Genome		Prestwick-6-E-2,
Screening Library		Selleck-6-D-7,
		Spectrum-2-H-5
MicroSource		01500282
Pharmakon		
MicroSource		01500282
Spectrum		
MicroSource US		01500282
Drugs		
MLSMR		144089058, 26719683, 56422158, 8139865
NIH Clinical		MLS001247032
Collection		
Prestwick Chemical		Prestw-441
SMDC Iconix		285659

Activities based on ChEMBL 20

View All 15 Activities

228 Total Observations

Gene Name	Class / Organism	pKi (L.E.)	Observations
ESR1: Estrogen receptor	Transcription factor / NR 	11.00 (0.77)	103
ESR2: Estrogen receptor beta	Transcription factor / NR 	11.00 (0.77)	94
AR: Androgen receptor	Transcription factor / NR 	7.72 (0.54)	6
AOX1: Aldehyde oxidase	enzyme / enzyme-other 	7.10 (0.50)	4
GPER1: G-protein coupled estrogen receptor 1	membrane receptor / GPCR-A 	9.52 (0.67)	4

SEA Predictions based on ChEMBL 20

View All 14

Run SEA

Gene	Description	Target Class	P-Value	Max Tc
Q95MF8_PIG	Sulfotransferase	enzyme / enzyme- other	0	67
SLCO1A1	Solute carrier organic anion transporter family member 1A1	Unclassified / unclassified	0	69
SULT1A1	Sulfotransferase 1A1	enzyme / enzyme- other	0	58
HSD17B2	Estradiol 17-beta- dehydrogenase 2	enzyme / enzyme- other	0	56
NR3C2	Mineralocorticoid receptor	Transcription factor / NR	0	49

### Interesting Analogs

[Find All](#)

### Endogenous

[Find More ➡](#)

#### None Found

Similar Endogenous

Run search for more

### Metabolites

Find More ➔

**None Found**  
Similar Metabolites

Run search for more

### Natural Products

Find More ➡

**None Found**

Similar Natural Products

Run search for more

### Aggregators

Find More ➡

**None Found**  
Similar Aggregators

Run search for more

## Drugs

Find More ➔

**None Found**  
Similar World Drugs

Run search for more

In-Man

Find More ➡

**None Found**

Similar In-Man



Run search for more

### Bioactives

Find More ➡

**None Found**  
Similar Bioactives

Run search for more

### Purchasable

Find More ➔

**Not Computed**

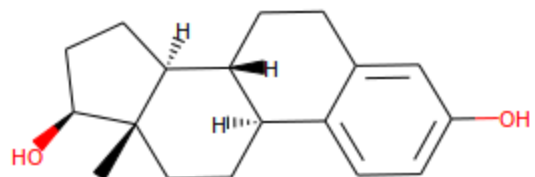
Should take ~10s

Run search for more

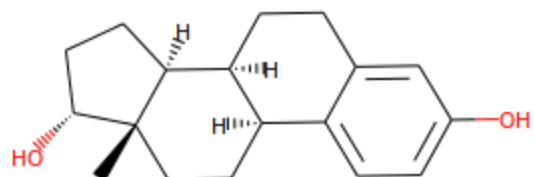
### Framework of this compound

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# ZINC13520815



3875384



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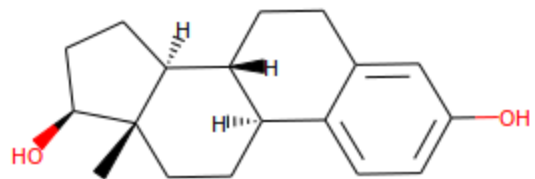
## Scaffold of this Compound



**GBGFUQOSVTZLFA-UHFFFAOYSA-N**

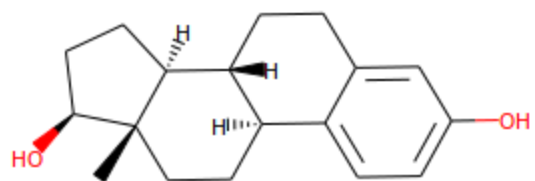
## Substance Rings

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7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene

### Molecular Patterns (Warnings, etc.)



**alcohol-secondary**  
reagent**References**[View All 97](#)

<b>Doc</b>	<b>Year</b>	<b>Journal</b>	<b>Volume</b>	<b>Issue</b>	<b>Pages</b>	<b><u>Link</u></b>
59306					–	CHEMBL1909046
91333	2015	J. Med. Chem.	58	3	1184–1194	25559213
76383	2014	Bioorg. Med. Chem.	22	1	303–310	24315190
89585	2014	Bioorg. Med. Chem. Lett.	24	22	5265–5267	25305688
89676	2014	J. Med. Chem.	57	22	9370–9382	25369367

**Clinical Trials**[View All 1202](#)

Trial ID	Title	Status	Phase	Start Date	Changed Date	Condition(s)	Drug(s)
NCT00029757	Buccal Estrogen in Toothpaste Study: Systemic Absorption of Estradiol When Administered Mixed With Toothpaste in Postmenopausal or Surgically Menopausal Women	Completed		Unknown	2005-11-04		Estradiol Estrogens



Trial ID	Title	Status	Phase	Start Date	Changed Date	Condition(s)	Drug(s)
NCT00044837	Hormone Replacement Therapy and Anti-HIV Drugs in HIV-Infected, Postmenopausal Women	Terminated	Phase 1	Unknown	2015-06-03	HIV Infections	Hormones Estradiol Polyestradiol phosphate Ritonavir Lopinavir Efavirenz Estradiol 3-benzoate Estradiol 17 beta-cypionate Estradiol valerate Medroxyprogesterone Medroxyprogesterone Acetate

Trial ID	Title	Status	Phase	Start Date	Changed Date	Condition(s)	Drug(s)
NCT00125983	Drug Interactions Between Lopinavir/Ritonavir and Oral or Patch Contraceptives in HIV Infected Women	Completed	Phase 2	Unknown	2012-05-17	HIV Infections	Ritonavir Lopinavir Contraceptive Agents Ortho Evra Norinyl Norethindrone acetate, ethinyl estradiol, ferrous fumarate drug combination Contraceptives, Oral
NCT00160173	Efficacy Study Comparing 0.9 g and 1.25 g Estrogel With Placebo for Vasomotor Symptoms and Vulvar and Vaginal Atrophy	Completed	Phase 4	Unknown	2013-07-11	Atrophy	Estradiol

Trial ID	Title	Status	Phase	Start Date	Changed Date	Condition(s)	Drug(s)
NCT00248963	Study Evaluating Levonorgestrel and Ethinyl Estradiol in Oral Contraception	Completed	Phase 3	Unknown	2006-05-17		Estradiol Polyestradiol phosphate Ethinyl Estradiol Estradiol 3-benzoate Estradiol 17 beta-cypionate Estradiol valerate Contraceptive Agents Levonorgestrel Ethinyl estradiol, levonorgestrel drug combination Contraceptives, Oral

#### Additional Identifiers (Synonyms/CAS Numbers/etc.)

<b>CAS Numbers</b>	50-28-2 , 35380-71-3
<b>ATC Code(s)</b>	G03CA03 , G03CA53
<b>WHO Name(s)</b>	estradiol , estradiol, combinations
<b>Molecule Names</b>	ESTRADIOL
<b>Synonyms</b>	Estradiol

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[Irwin and Shoichet Labs](#) and [UC Regents](#).

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