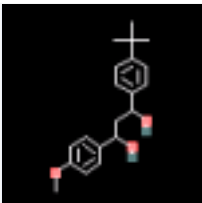
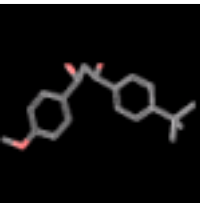


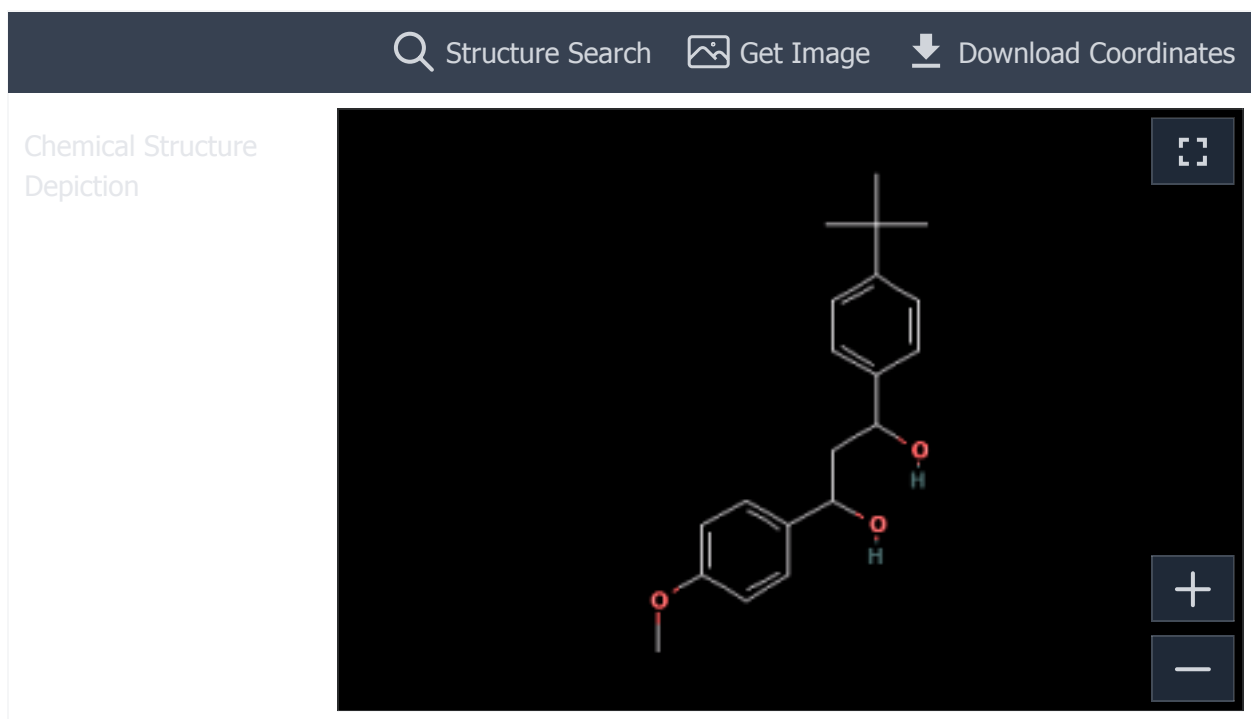


COMPOUND SUMMARY

1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)1,3-propanediol

PubChem CID	12091724
Structure	  2D 3D
Chemical Safety	  Irritant Environmental Hazard Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{20}H_{26}O_3$
Synonyms	1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)1,3-propanediol 955359-35-0 1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)-1,3-propanediol 1-(4-(tert-Butyl)phenyl)-3-(4-methoxyphenyl)propane-1,3-diol 1-(4-tert-butylphenyl)-3-(4-methoxyphenyl)propane-1,3-diol View More...
Molecular Weight	314.4 g/mol <i>Computed by PubChem 2.1 (PubChem release 2021.05.07)</i>
Dates	Create: 2007-02-07 Modify: 2024-09-28

1.1 2D Structure



▶ PubChem

1.2 3D Conformer



▶ PubChem

2 Names and Identifiers



2.1 Computed Descriptors



2.1.1 IUPAC Name



1-(4-*tert*-butylphenyl)-3-(4-methoxyphenyl)propane-1,3-diol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

▶ [PubChem](#)

2.1.2 InChI



InChI=1S/C20H26O3

/c1-20(2,3)16-9-5-14(6-10-16)18(21)13-19(22)15-7-11-17(23-4)12-8-15

/h5-12,18-19,21-22H,13H2,1-4H3

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

▶ [PubChem](#)

2.1.3 InChIKey



GTIRDWBOUTYFQO-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

▶ [PubChem](#)

2.1.4 SMILES



CC(C)(C)C1=CC=C(C=C1)C(CC(C2=CC=C(C=C2)OC)O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

▶ [PubChem](#)

2.2 Molecular Formula



C₂₀H₂₆O₃

Computed by PubChem 2.1 (PubChem release 2021.05.07)

▶ [PubChem](#)

2.3 Other Identifiers



2.3.1 CAS



[955359-35-0](#)

- ▶ [CAS Common Chemistry](#); [EPA DSSTox](#); [European Chemicals Agency \(ECHA\)](#)

2.3.2 European Community (EC) Number



[943-286-0](#)

- ▶ [European Chemicals Agency \(ECHA\)](#)

2.3.3 DSSTox Substance ID



[DTXSID701019370](#)

- ▶ [EPA DSSTox](#)

2.3.4 Nikkaji Number



[J3.426.443K](#)

- ▶ [Japan Chemical Substance Dictionary \(Nikkaji\)](#)

2.4 Synonyms



2.4.1 Depositor-Supplied Synonyms



[1-\(4-tert-Butylphenyl\)-3-\(4-methoxyphenyl\)1,3-propanediol](#)
[955359-35-0](#)
[1-\(4-tert-Butylphenyl\)-3-\(4-methoxyphenyl\)-1,3-propanediol](#)
[1-\(4-\(tert-Butyl\)phenyl\)-3-\(4-methoxyphenyl\)propane-1,3-diol](#)
[1-\(4-tert-butylphenyl\)-3-\(4-methoxyphenyl\)propane-1,3-diol](#)
[AVOBENZONE_met016](#)
[SCHEMBL5234821](#)
[GTIRDWBOUTYFQO-UHFFFAOYSA-N](#)
[DTXSID701019370](#)
[AKOS015998744](#)

[▶ PubChem](#)

3 Chemical and Physical Properties



3.1 Computed Properties



Property Name	Property Value	Reference
Molecular Weight	314.4 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	3.9	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	6	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	314.18819469 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	314.18819469 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	49.7Å ²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	333	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	2	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem

Property Name	Property Value	Reference
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

▶ [PubChem](#)

3.2 Experimental Properties



3.2.1 Collision Cross Section



171.06 Å² [M+Na]⁺ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

Ross et al. JASMS 2022; 33; 1061-1072. DOI:10.1021/jasms.2c00111

▶ [CCSbase](#)

4 Related Records



4.1 Related Compounds with Annotation



Follow these links to [do a live 2D search](#) or [do a live 3D search](#) for this compound, sorted by annotation score. This section is deprecated (see [here](#) for details), but these live search links provide equivalent functionality to the table that was previously shown here.

▶ [PubChem](#)

4.2 Related Compounds



Same Connectivity Count	5
Same Parent, Connectivity Count	5
Mixtures, Components, and	2

Neutralized Forms Count	
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

▶ [PubChem](#)

4.3 Substances



4.3.1 Related Substances



All Count	38
Same Count	36
Mixture Count	2

▶ [PubChem](#)

4.3.2 Substances by Category



▶ [PubChem](#)

5 Chemical Vendors





▶ [PubChem](#)

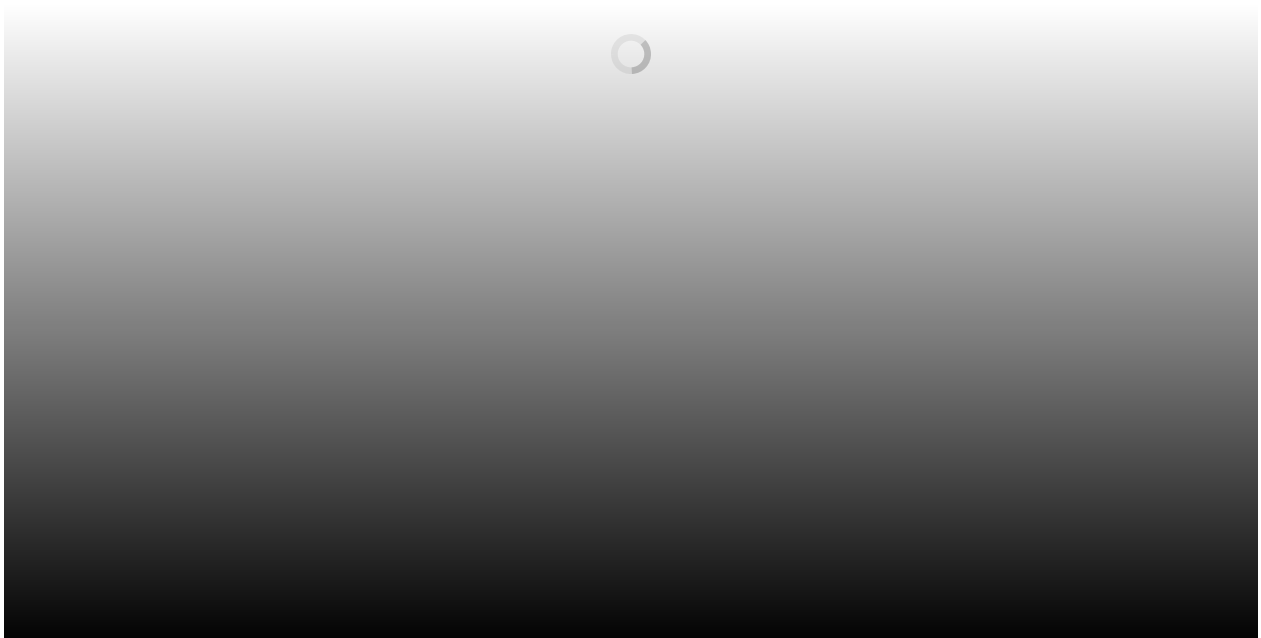
6 Use and Manufacturing



6.1 Uses



EPA CPDat Chemical and Product Categories



The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

▶ [EPA Chemical and Products Database \(CPDat\)](#)

7 Safety and Hazards



7.1 Hazards Identification



7.1.1 GHS Classification



Pictogram(s)	<p>Irritant Environmental Hazard</p>
Signal	<u>Warning</u>
GHS Hazard Statements	H315 (100%): Causes skin irritation [<u>Warning</u> Skin corrosion/irritation] H411 (100%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P264, P273, P280, P302+P352, P321, P332+P317, P362+P364, P391, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	<i>The GHS information provided by 1 company from 1 notification to the ECHA C&L Inventory.</i>

▶ [European Chemicals Agency \(ECHA\)](#)

7.1.2 Hazard Classes and Categories



Skin Irrit. 2 (100%)

Aquatic Chronic 2 (100%)

▶ [European Chemicals Agency \(ECHA\)](#)

7.2 Regulatory Information



REACH Registered Substance

Status: Active Update: 08-12-2017 <https://echa.europa.eu/registration-dossier/-/registered-dossier/21538>

▶ [European Chemicals Agency \(ECHA\)](#)

8 Literature



8.1 Consolidated References



1 item

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Ross et al. JASMS 2022; 33; 1061-1072. DOI:10.1021/jasms.2c00111

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9 Patents



9.1 Depositor-Supplied Patent Identifiers



31 items

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Priority Date - Most Recent

[Compositions of fluorinated surfactants and antioxidants](#)

Publication Number: [EP-3322400-A1](#)

Priority Date: 2015-07-14

[Compositions of fluorinated surfactants and antioxidants](#)

Publication Number: [US-2018207080-A1](#)

Priority Date: 2015-07-14

[Compositions of fluorinated surfactants and antioxidants](#)

Publication Number: [WO-2017008877-A1](#)

Priority Date: 2015-07-14

[Mixtures of creatine or creatinine and glucuronolactones](#)

Publication Number: [WO-2015078554-A1](#)

Priority Date: 2013-11-26

[Glucuronolactone derivatives as self-tanning substances](#)

Publication Number: [EP-2958925-A1](#)

Priority Date: 2013-02-25

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 Last

[▶ PubChem](#)

[Link to all deposited patent identifiers](#)[▶ PubChem](#)

9.2 WIPO PATENTSCOPE

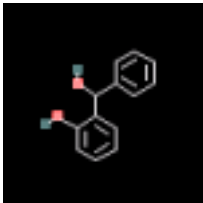
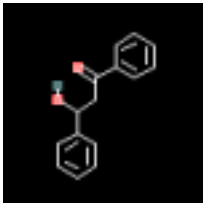
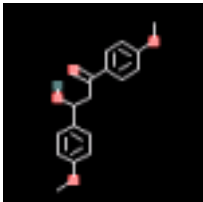


Patents are available for this chemical structure:

<https://patentscope.wipo.int/search/en/result.jsf?inchikey=GTIRDWBOUTYFQO-UHFFFAOYSA-N>[▶ PATENTSCOPE \(WIPO\)](#)

9.3 Chemical Co-Occurrences in Patents

Showing 3 of 15 [View More Co-Occurrence and Evidence Data](#)[Download](#)

Chemical	Selected evidence
 <p>2-[Hydroxy(phenyl)methyl]phenol CID 2751543</p>	<p>1 patent from 1 patent family View All</p> <p>Antioxidants EP-2010294-B1; Grant Date: 2015-12-02</p>
 <p>3-Hydroxy-1,3-diphenylpropan-1-one CID 10059587</p>	<p>1 patent from 1 patent family View All</p> <p>Antioxidants EP-2010294-B1; Grant Date: 2015-12-02</p>
 <p>3-Hydroxy-1,3-bis(4-</p>	<p>1 patent from 1 patent family View All</p> <p>Antioxidants EP-2010294-B1; Grant Date: 2015-12-02</p>

Chemical	Selected evidence
methoxyphenyl)-1-propanone CID 11778741	

▶ [PubChem](#)

9.4 Chemical-Disease Co-Occurrences in Patents



Showing 3 of 33 View More Co-Occurrence and Evidence Data		Download
Disease	Selected evidence	
Skin Diseases	1 patent from 1 patent family	View All
	Antioxidants EP-2010294-B1; Grant Date: 2015-12-02	
Gingival Hypertrophy	1 patent from 1 patent family	View All
	Antioxidants EP-2010294-B1; Grant Date: 2015-12-02	
Epidermodysplasia Verruciformis	1 patent from 1 patent family	View All
	Antioxidants EP-2010294-B1; Grant Date: 2015-12-02	

▶ [PubChem](#)

9.5 Chemical-Gene Co-Occurrences in Patents



Showing 1 of 1 View More Co-Occurrence and Evidence Data		Download
Gene	Selected evidence	
insulin	1 patent from 1 patent family	View All
	Antioxidants EP-2010294-B1; Grant Date: 2015-12-02	

[▶ PubChem](#)

10 Classification



10.1 UN GHS Classification



15 items

[View in Classification Browser](#)

GHS Classification Tree > Hazard Statement Codes > H300: Health Hazards
H315: Causes skin irritation [Warning Skin corrosion/irritation]

GHS Classification Tree > Hazard Statement Codes > H400: Environmental Hazards
H411: Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

GHS Classification Tree > Hazard Classes > Environmental Hazards
Hazardous to the aquatic environment, long-term hazard

GHS Classification Tree > Hazard Classes > Health Hazards
Skin corrosion/irritation

GHS Classification Tree > Hazard Pictograms



GHS07

« First < Previous Page 1 of 3 Next > Last »

[▶ GHS Classification \(UNECE\)](#)

10.2 EPA CPDat Classification



1 item

[View in Classification Browser](#)

EPA CPDat Classification > Functional Use > Reported Functional Use
skin conditioning

[▶ EPA Chemical and Products Database \(CPDat\)](#)

10.3 NORMAN Suspect List Exchange Classification



1 item

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NORMAN Suspect List Exchange Classification

S112 | FCCMIGEX | List of Migrating & Extractable Food Contact Chemicals (FCCmigex) by FPF

List of migrating and extractable food contact chemicals (FCCmigex) systematically compiled as a database using information from over 1300 studies under the ongoing Food Contact Chemicals and Human Health (FCCH) Project led by the Food Packaging Forum. A peer-reviewed, open-access article (Geueke et al. 2023, DOI:<https://doi.org/10.1080/10408398.2022.2067828>) contains detailed information about compilation of the FCCmigex database which includes more than 4,000 food contact chemicals and over 24,000 database entries, browseable at <https://www.foodpackagingforum.org/fccmigex>. The list was kindly provided by Birgit Geueke & Lindsey Parkinson

▶ [NORMAN Suspect List Exchange](#)

10.4 CCSBase Classification



1 item

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CCSbase Classification

[M+Na]⁺

▶ [CCSbase](#)

10.5 EPA DSSTox Classification



▶ [EPA DSSTox](#)

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1-[4-(1,1-Dimethylethyl)phenyl]-3-(4-methoxyphenyl)-1,3-propanediol

https://commonchemistry.cas.org/detail?cas_rn=955359-35-0

2. EPA DSSTox

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<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)-1,3-propanediol

<https://comptox.epa.gov/dashboard/DTXSID701019370>

CompTox Chemicals Dashboard Chemical Lists

<https://comptox.epa.gov/dashboard/chemical-lists/>

3. European Chemicals Agency (ECHA)

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<https://echa.europa.eu/web/guest/legal-notice>

1-(4-tert-Butyl-phenyl)-3-(4-methoxy-phenyl)-propane-1,3-diol

<https://chem.echa.europa.eu/100.243.100>

1-(4-tert-Butyl-phenyl)-3-(4-methoxy-phenyl)-propane-1,3-diol (EC: 943-286-0)

<https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/250687>

4. CCSbase

CCSbase Classification

<https://ccsbase.net/>

5. EPA Chemical and Products Database (CPDat)

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<https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources>

1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)-1,3-propanediol

<https://comptox.epa.gov/dashboard/DTXSID701019370#exposure>

EPA CPDat Classification

<https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>

6. Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.426.443K

7. PubChem

<https://pubchem.ncbi.nlm.nih.gov>

8. GHS Classification (UNECE)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

9. NORMAN Suspect List Exchange

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NORMAN Suspect List Exchange Classification

<https://www.norman-network.com/nds/SLE/>

10. PATENTSCOPE (WIPO)

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<https://pubchem.ncbi.nlm.nih.gov/substance/391829320>

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