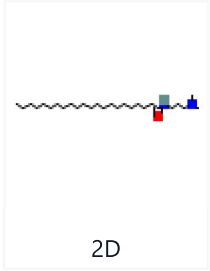
PubChem

COMPOUND SUMMARY

Behenamidopropyl Dimethylamine

Cite | Download

PubChem CID	108912
Structure	 2D
Chemical Safety	 Corrosive Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{27}H_{56}N_2O$
Synonyms	Behenamidopropyl dimethylamine 60270-33-9 n-[3-(dimethylamino)propyl]docosanamide amidet N-(3-(Dimethylamino)propyl)docosanamide

View More...

Molecular Weight	424.7 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-08-08 Modify: 2025-04-12

Contents

1 Structures

1.1 2D Structure

Chemical Structure Depiction

PubChem

1.2 3D Status

Conformer generation is disallowed since too flexible

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

N-[3-(dimethylamino)propyl]docosanamide

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▸ PubChem

2.1.2 InChI

InChI=1S/C27H56N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-27(30)28-25-23-26-29(2)3/h4-26H2,1-3H3,(H,28,30)

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

2.1.3 InChIKey

MNAZHGAWPCLLGX-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

2.1.4 SMILES

CCCCCCCCCCCCCCCCCCCCCC(=O)NCCCN(C)C

Computed by OEChem 2.3.0 (PubChem release 2024.12.12)

▸ PubChem

2.2 Molecular Formula

$C_{27}H_{56}N_2O$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

▸ Australian Industrial Chemicals Introduction Scheme (AICIS); PubChem

2.3 Other Identifiers

2.3.1 CAS

60270-33-9

▸ Australian Industrial Chemicals Introduction Scheme (AICIS); CAS Common Chemistry; ChemIDplus; EPA DSSTox; European Chemicals A…

2.3.2 European Community (EC) Number

262-134-8

▸ European Chemicals Agency (ECHA)

2.3.3 UNII

X4O854526J

- FDA Global Substance Registration System (GSRS)

2.3.4 DSSTox Substance ID

DTXSID90209025

- EPA DSSTox

2.3.5 Nikkaji Number

J298.809G

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.6 Wikidata

Q27293552

- Wikidata

2.4 Synonyms

2.4.1 MeSH Entry Terms

amidet
APA 22

APA-22
APA22 cpd
N-(3-(dimethylamino)propyl)docosanamide
N-(3-(dimethylamino)propyl)docosanamide chloride

▸ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Behenamidopropyl dimethylamine
60270-33-9
n-[3-(dimethylamino)propyl]docosanamide
amidet
N-(3-(Dimethylamino)propyl)docosanamide
Dimethylaminopropyl behenamide
UNII-X4O854526J
INCROMINE BD
behenic acid dimethylaminopropylamide
EINECS 262-134-8
AMIDET APA-22
MACKINE 601
NIKKOL AMIDOAMINE MPB
Docosanamide, N-[3-(dimethylamino)propyl]-
DTXSID90209025
X4O854526J
N',N'-DIMETHYL-N-DOCOSANOYL-1,3-DIAMINOPROPANE
Docosanamide,N-[3-(dimethylamino)propyl]-
DOCOSANAMIDE, N-(3-(DIMETHYLAMINO)PROPYL)-
APA22 cpd
SCHEMBL74161
APA 22
APA-22
DTXCID10131516
N-3-Erucylamidopropyl dimethyla
N-[3-(dimethylamino)propyl]doc
DB-266024
BEHENAMIDOPROPYL DIMETHYL
NS00013392
N-(3-(dimethylamino)propyl)doco

▸ PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference

Molecular Weight	424.7 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3-AA	10.5	Computed by XLogP3 3.0 (PubChem release 2021.10.14)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	24	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	424.439264414 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	424.439264414 Da	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	32.3 $Å^2$	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	30	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	344	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem

Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

▸ PubChem

3.2 Chemical Classes

3.2.1 Cosmetics

Cosmetic ingredients (Behenamidopropyl Dimethylamine) -> CIR (Cosmetic Ingredient Review)

▸ Cosmetic Ingredient Review (CIR)

Antistatic; Emulsifying

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | DOI:10.5281/zenodo.2624118

▸ NORMAN Suspect List Exchange

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 Parent, Exact Count	11
Mixtures, Components, and Neutralized Forms Count	16
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

4.3 Substances

4.3.1 PubChem Reference Collection SID

500760298

PubChem

4.3.2 Related Substances

All Count	114
Same Count	53
Mixture Count	61

PubChem

4.3.3 Substances by Category

PubChem

4.4 Entrez Crosslinks

PubMed Count	2

PubChem

5 Chemical Vendors

▸ PubChem

6 Use and Manufacturing

6.1 Uses

Cosmetic Ingredient Review Link

CIR ingredient: Behenamidopropyl Dimethylamine

▸ Cosmetic Ingredient Review (CIR)

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)**

6.1.1 Use Classification

Cosmetics -> Antistatic; Emulsifying

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | ***DOI:10.5281/zenodo.2624118***

▸ **NORMAN Suspect List Exchange**

6.1.2 Household Products

Household & Commercial/Institutional Products

Information on 16 consumer products that contain Behenamidopropyl dimethylamine in the following categories is provided:

• Personal Care

▸ Consumer Product Information Database (CPID)

7 Safety and Hazards

7.1 Hazards Identification

7.1.1 GHS Classification

1 of 2 View All

Pictogram(s)	 Corrosive Irritant
Signal	**Danger**
GHS Hazard Statements	H315 (55.4%): Causes skin irritation [**Warning** Skin corrosion/irritation] H318 (77.1%): Causes serious eye damage [**Danger** Serious eye damage/eye irritation] H319 (21.7%): Causes serious eye irritation [**Warning** Serious eye damage/eye irritation] H412 (24.1%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P264, P264+P265, P273, P280, P302+P352, P305+P351+P338, P305+P354+P338, P317, P321, P332+P317, P337+P317, P362+P364, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided per 83 reports by companies from 7 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that*

*provide hazard codes. Only hazard codes with percentage values above 10% are shown. For more detailed information, please visit **ECHA C&L website.***

▸ European Chemicals Agency (ECHA)

7.1.2 Hazard Classes and Categories

Skin Irrit. 2 (55.4%)

Eye Dam. 1 (77.1%)

Eye Irrit. 2A (21.7%)

Aquatic Chronic 3 (24.1%)

▸ European Chemicals Agency (ECHA)

Skin corrosion - category 1

Skin sensitisation - category 1B

▸ Hazardous Chemical Information System (HCIS), Safe Work Australia

7.2 Regulatory Information

The Australian Inventory of Industrial Chemicals

Chemical: Docosanamide, N-[3-(dimethylamino)propyl]-

▸ Australian Industrial Chemicals Introduction Scheme (AICIS)

REACH Registered Substance

Status: Active Update: 12-04-2023 https://echa.europa.eu/registration-dossier/-/registered-dossier/16782

- European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

Docosanamide, N-3-(dimethylamino)propyl-: Does not have an individual approval but may be used under an appropriate group standard

- New Zealand Environmental Protection Authority (EPA)

7.3 Other Safety Information

Chemical Assessment

IMAP assessments - Fatty acid amido propyl dimethylamines: Human health tier II assessment

- Australian Industrial Chemicals Introduction Scheme (AICIS)

8 Literature

8.1 Consolidated References

PubChem

8.2 NLM Curated PubMed Citations

PubChem

8.3 Springer Nature References

▸ Springer Nature

8.4 Chemical Co-Occurrences in Literature

▸ PubChem

8.5 Chemical-Gene Co-Occurrences in Literature

▸ PubChem

8.6 Chemical-Disease Co-Occurrences in Literature

PubChem

9 Patents

9.1 Depositor-Supplied Patent Identifiers

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=MNAZHGAWPCLLGX-UHFFFAOYSA-N

▸ PATENTSCOPE (WIPO)

9.3 Chemical Co-Occurrences in Patents

▸ PubChem

9.4 Chemical-Disease Co-Occurrences in Patents

PubChem

9.5 Chemical-Gene Co-Occurrences in Patents

PubChem

10 Classification

10.1 MeSH Tree

Medical Subject Headings (MeSH)

10.2 ChemIDplus

- ChemIDplus

10.3 Household Products Database Tree

- Consumer Product Information Database (CPID)

10.4 UN GHS Classification

▸ GHS Classification (UNECE)

10.5 EPA CPDat Classification

▸ EPA Chemical and Products Database (CPDat)

10.6 NORMAN Suspect List Exchange Classification

▸ NORMAN Suspect List Exchange

10.7 EPA DSSTox Classification

▸ EPA DSSTox

10.8 Consumer Product Information Database Classification

- Consumer Product Information Database (CPID)

10.9 MolGenie Organic Chemistry Ontology

- MolGenie

10.10 Chemicals in PubChem from Regulatory Sources

▸ PubChem

11 Information Sources

FILTER BY SOURCE

ALL SOURCES

1. ### Australian Industrial Chemicals Introduction Scheme (AICIS)

   LICENSE
   https://www.industrialchemicals.gov.au/copyright

   Docosanamide, N-[3-(dimethylamino)propyl]-
   https://services.industrialchemicals.gov.au/search-assessments/

   Docosanamide, N-[3-(dimethylamino)propyl]-
   https://services.industrialchemicals.gov.au/search-inventory/

2. ### CAS Common Chemistry

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   Behenic acid dimethylaminopropylamide
   https://commonchemistry.cas.org/detail?cas_rn=60270-33-9

3. ### ChemIDplus

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https://www.nlm.nih.gov/copyright.html

Behenamidopropyl dimethylamine

https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0060270339

ChemIDplus Chemical Information Classification

https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

4. EPA DSSTox

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

N-[3-(Dimethylamino)propyl]docosanamide

https://comptox.epa.gov/dashboard/DTXSID90209025

CompTox Chemicals Dashboard Chemical Lists

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

5. European Chemicals Agency (ECHA)

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

N-[3-(dimethylamino)propyl]docosanamide

https://chem.echa.europa.eu/100.056.468

N-[3-(dimethylamino)propyl]docosanamide (EC: 262-134-8)

https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/80654

6. FDA Global Substance Registration System (GSRS)

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https://www.fda.gov/about-fda/about-website/website-policies#linking

BEHENAMIDOPROPYL DIMETHYLAMINE

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/X4O854526J

7. New Zealand Environmental Protection Authority (EPA)

Docosanamide, N-3-(dimethylamino)propyl-

https://www.epa.govt.nz/industry-areas/hazardous-substances/guidance-for-importers-and-manufacturers/hazardous-substances-databases/

8. Consumer Product Information Database (CPID)

Behenamidopropyl dimethylamine

https://www.whatsinproducts.com/chemicals/view/1/3682/060270-33-9

Household Products Classification

https://hpd.nlm.nih.gov/

Consumer Products Category Classification

https://www.whatsinproducts.com/

9. Cosmetic Ingredient Review (CIR)

Behenamidopropyl Dimethylamine

https://cir-reports.cir-safety.org/cir-ingredient-status-report/?id=1a964f74-9934-4ab4-b026-dce544166be5

10. EPA Chemical and Products Database (CPDat)

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

https://comptox.epa.gov/dashboard/DTXSID90209025#exposure

EPA CPDat Classification

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

11. ## NORMAN Suspect List Exchange

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NORMAN Suspect List Exchange Classification

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

12. ## Hazardous Chemical Information System (HCIS), Safe Work Australia

60270-33-9

http://hcis.safeworkaustralia.gov.au/HazardousChemical/Details?chemicalID=6766

13. ## Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J298.809G

14. ## Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/341681962

15. ## Wikidata

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https://www.wikidata.org/wiki/Q27293552

16. PubChem

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

17. Medical Subject Headings (MeSH)

N-(3-(dimethylamino)propyl)docosanamide

https://www.ncbi.nlm.nih.gov/mesh/67533672

MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

18. GHS Classification (UNECE)

GHS Classification

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

19. MolGenie

MolGenie Organic Chemistry Ontology

https://github.com/MolGenie/ontology/

20. PATENTSCOPE (WIPO)

SID 388453745

https://pubchem.ncbi.nlm.nih.gov/substance/388453745