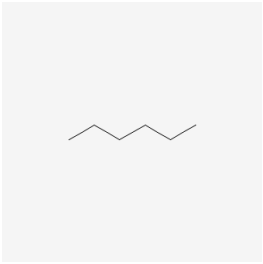
Technical Data Sheet

Hexane ACS Reagent Grade

ACS Reagent

Alliance Code	Revised	Revision
hexane-acs-reagent-grade	2026-10-13	1.6

CAS number 110-54-3	UN number UN1208	Hazard class · packing group 3 · PG II
 Structure · PubChem	Grade ACS Reagent	Signal word **Danger**

Hazards

Flammable | Irritant / harmful | Health hazard | Environmental hazard

H225 H304 H315 H336 H361f H373 H411

Proper shipping name
Hexanes

IDENTITY & COMPOSITION

PRODUCT NAME
Hexane ACS Reagent Grade

ALLIANCE CODE
hexane-acs-reagent-grade

GRADE
ACS Reagent

CONCENTRATION
—

CAS NUMBER
110-54-3 PubChem

FORMULA
C6H14 PubChem

MOLECULAR WEIGHT
86.18 PubChem

PRODUCT TYPE
Pure substance

SPECIFICATIONS

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Assay (sum of 5 isomers, total hexanes, plus methylcyclopentane)	min. 98.5 %	—	Gas chromatography (GC)	Interpreted
Color (APHA)	10 max.	—	—	Interpreted
n-Hexane	45.0% min.	—	—	Interpreted
Residue After Evaporation	0.001% max.	—	—	Interpreted
Sulfur Compounds (as S)	0.005% max.	—	—	Interpreted
Thiophene	To Pass Test	—	—	Interpreted
Water Soluble Titratable Acid	0.0003 meq/g max.	—	—	Interpreted
Substances Darkened by Sulfuric Acid	To Pass Test	—	ACS monograph procedure (sulfuric acid shake test), visual comparison	Interpreted
Distillation Range	62 - 70 C	—	ASTM D1078	Interpreted

Values are reproduced from the current product reference. Source labels do not by themselves establish a supplier guarantee or a test result for your lot. Confirm applicable acceptance limits and request lot-specific documentation.

AVAILABLE GRADES SAME CAS, ALTERNATE GRADES AND CONCENTRATIONS

GRADE	CONCENTRATION	TYPICAL ASSAY	SKU
THIS GRADE ACS Reagent	—	—	current
Technical Grade	—	—	hexane-technical-grade-1

Typical assay for each grade is the average of its recent lots. Confirm a grade meets your specification before substituting it.

PHYSICAL & CHEMICAL PROPERTIES

PROPERTY	VALUE	SOURCE
Appearance	Clear, volatile light hydrocarbon liquid	Adjudicated
Form	Liquid	Published reference
Odor	Gasoline-like (petroleum distillate) odor	Adjudicated
Specific Gravity	0.659 at 25 °C (water = 1)	Adjudicated
Density	0.659 at 68 °F (USCG, 1999) - Less dense than water; will float	Published reference
Boiling Point	69 °C (156 °F) at 760 mmHg	Adjudicated
Melting Point	-95 °C (-139 °F)	Adjudicated
Flash Point	-22 °C (-8 °F), closed cup	Adjudicated
Vapor Pressure	160–176 hPa (120–132 mmHg) at 20 °C	Adjudicated
Vapor Density	2.97 (air = 1)	Adjudicated
Solubility (water)	Practically insoluble in water (about 0.01 g/L)	Adjudicated
Refractive Index (nD 20)	1.372 - 1.380	Interpreted
Viscosity	0.31 mPa·s at 20 °C	Adjudicated

MATERIALS OF CONSTRUCTION SERVICE ENVELOPE ≈ 100%

MATERIAL	RATING	MAX T (°C)	NOTES	SOURCE
Buna-N (NBR) Elastomer	Good	80	Good for non-aromatic hydrocarbons; poor for aromatics.	Parker O-ring Chemical Compatibility
EPDM Elastomer	Not recommended	—	Swells in hydrocarbons; never use.	Parker O-ring Chemical Compatibility
Viton (FKM) Elastomer	Excellent	100	Standard for hydrocarbon service.	Parker O-ring Chemical Compatibility
PTFE Fluoropolymer	Excellent	200	Universal.	Cole-Parmer Chemical Compatibility
316L Stainless Steel Metal	Excellent	100	Inert.	Cole-Parmer Chemical Compatibility
Carbon Steel Metal	Good	80	Acceptable for dry hydrocarbons.	Cole-Parmer Chemical Compatibility
HDPE Thermoplastic	Not recommended	—	Unsatisfactory even at room temperature.	INEOS HDPE Chemical Resistance Guide

Ratings reflect the service envelope (concentration × temperature) shown. Always confirm against your specific duty cycle and contact-time before equipment selection. The most cautious rating across overlapping references is shown.

REGULATORY & TRANSPORT

DOT / 49 CFR

UN NUMBER

UN1208 49 CFR 172.101

HAZARD CLASS

3 Adjudicated

PACKING GROUP

II Adjudicated

PROPER SHIPPING NAME

Hexanes Adjudicated

GHS / OSHA HCS 2024

SIGNAL WORD

Danger Adjudicated

H-CODES (HAZARD STATEMENTS)

H225, H304, H315, H336, H361f, H373, H411

ECHA C&L Inventory

P-CODES (PRECAUTIONARY STATEMENTS)

P201, P202, P210, P233, P240, P241, P242, P243, P260, P261, P264, P270, P271, P273, P280, P301+P310, P302+P352, P303+P361+P353, P304+P340, P308+P313, P312, P314, P321, P331, P332+P313, P362, P370+P378, P391, P403+P233, P403+P235, P405, P501

ECHA C&L Inventory

OCCUPATIONAL EXPOSURE LIMITS

OSHA PEL (29 CFR 1910.1000)

500 ppm TWA OSHA 29 CFR 1910.1000

ACGIH TLV

50 ppm TWA (skin notation: absorbed through the skin)

Adjudicated

NIOSH REL

50 ppm TWA NIOSH Pocket Guide

NIOSH IDLH

1100 ppm (10% LEL) NIOSH Pocket Guide

Transport descriptions reflect 49 CFR 172.101 lookup at time of publication. Sourced data: NIOSH Pocket Guide for REL/IDLH, OSHA Z-Tables for PEL. Always verify against the latest regulatory text before shipment-critical decisions.

HEALTH & FIRE HAZARD

ACUTE TOXICOLOGY

LD_{50} ORAL (RAT)

25,000 mg/kg Adjudicated

LD_{50} DERMAL (RABBIT)

3,000 mg/kg Adjudicated

LC_{50} INHALATION (RAT, 4 H)

48,000 ppm (vapor)

Adjudicated

Acute toxicology values from SDS Section 11 or NIOSH RTECS.

CATALOG EQUIVALENTS CROSS-REFERENCE VS MAJOR CHEMICAL SUPPLIERS

SIGMA-ALDRICH

SKU	GRADE	CONC.	MATCH	NOTES
139386	ACS Reagent	95%	Unverified candidate	ACS Reagent ≥95%
296090	ACS reagent	≥98.5%	Unverified candidate	Same ACS reagent grade n-hexane.

Cross-references are informational. Confirm against the manufacturer's current specification before substitution. Competitor trademarks are property of their respective owners.

APPLICATIONS

Laboratory and analytical solvent (ACS reagent): extraction, chromatography and spectroscopy. Adjudicated

Restrictions on Use: For industrial, professional and laboratory use. Do not use for cleaning or degreasing in poorly ventilated spaces: repeated n-hexane exposure damages the peripheral nerves.

STORAGE & HANDLING

RECOMMENDED STORAGE

Keep containers tightly closed in a cool, dry, well-ventilated flammables area away from heat, sparks, open flame and direct sunlight. Ground and bond containers when transferring. Protect from light.

Adjudicated

HANDLING PRECAUTIONS

Eliminate ignition sources. Use chemical-resistant nitrile or PVA gloves. Bond and ground all transfer equipment. Vapors heavier than air — control ventilation accordingly.

Class-level guidance — not product-specific; the SDS controls.

INCOMPATIBILITIES

Strong oxidizing agents; halogens (chlorine, fluorine) and halogen compounds.

Adjudicated

SHELF LIFE

Consult Technical Services for product-specific shelf life

For full hazard, PPE, and emergency response guidance, refer to the Safety Data Sheet (SDS) for this product. The SDS controls in all cases where guidance differs.

PACKAGING & LOGISTICS

SHIPPING DESCRIPTION (US DOT)

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UN1208, Hexanes, 3, PG II
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Sourced from 49 CFR 172.101. Confirm against shipping documents and carrier requirements before tender.

NMFC CLASS	PLACARD	PACKING GROUP
70	Flammable Liquid	PG II

REVISION HISTORY

Last reviewed 2026-10-13 by Andre Taki, Chief Commercial Officer, DOT Hazmat–certified (49 CFR 172.704).

VERSION	DATE	CHANGE	TRIGGER
1.6	2026-10-13	Canonical data updated: 1 field changed via the provenance/adjudication pipeline. • storage_precautions · canonical change (coa.data_provenance / adjudication)	canonical_change

VERSION	DATE	CHANGE	TRIGGER
1.5	2026-10-07	Canonical data updated: 20 fields changed via the provenance/adjudication pipeline. • synonyms · canonical change (coa.data_provenance / adjudication) • odor · canonical change (coa.data_provenance / adjudication) • flashPoint · canonical change (coa.data_provenance / adjudication) • boilingPoint · canonical change (coa.data_provenance / adjudication) • meltingPoint · canonical change (coa.data_provenance / adjudication) • vaporPressure · canonical change (coa.data_provenance / adjudication) • vaporDensity · canonical change (coa.data_provenance / adjudication) • specificGravity · canonical change (coa.data_provenance / adjudication) • solubility · canonical change (coa.data_provenance / adjudication) • viscosity · canonical change (coa.data_provenance / adjudication) • explosiveLimits · canonical change (coa.data_provenance / adjudication) • oel_acgih_tlv · canonical change (coa.data_provenance / adjudication) • incompatible_materials · canonical change (coa.data_provenance / adjudication) • conditions_to_avoid · canonical change (coa.data_provenance / adjudication) • hazardous_decomposition_products · canonical change (coa.data_provenance / adjudication) • rcra_waste_codes · canonical change (coa.data_provenance / adjudication) • cercla_rq · canonical change (coa.data_provenance / adjudication) • dot_transport_note · canonical change (coa.data_provenance / adjudication) • restrictions_on_use · canonical change (coa.data_provenance / adjudication) • recommended_use · canonical change (coa.data_provenance / adjudication)	canonical_change
1.4	2026-09-30	Canonical data updated: 4 fields changed via the provenance/adjudication pipeline. • boilingPoint · canonical change (coa.data_provenance / adjudication) • meltingPoint · canonical change (coa.data_provenance / adjudication) • flashPoint · canonical change (coa.data_provenance / adjudication) • appearance · canonical change (coa.data_provenance / adjudication)	canonical_change
1.3	2026-08-05	Canonical data updated: 4 fields changed via the provenance/adjudication pipeline. • hazardClass · canonical change (coa.data_provenance / adjudication) • packingGroup · canonical change (coa.data_provenance / adjudication) • signalWord · canonical change (coa.data_provenance / adjudication) • unNumber · canonical change (coa.data_provenance / adjudication)	canonical_change

VERSION	DATE	CHANGE	TRIGGER
1.2	2026-07-22	Canonical data updated: 2 fields changed via the provenance/adjudication pipeline. • dotSubsidiaryHazardClass · canonical change (coa.data_provenance / adjudication) • dotProperShippingName · canonical change (coa.data_provenance / adjudication)	canonical_change
1.1	2026-06-18	Canonical data re-verified: 3 fields updated against independent vendor SDSs, CLP Annex VI, 49 CFR, and OSHA HazCom 2024 (GHS classification, hazard/precautionary codes, signal word, physical properties as applicable). • countryOfOrigin · canonical adjudication / reground (coa.data_provenance) • ghsClassification · canonical adjudication / reground (coa.data_provenance) • hsCode · canonical adjudication / reground (coa.data_provenance)	canonical_change
1.0	2026-05-20	Initial URL-first TDS published from canonical chemistry registry.	initial

This Technical Data Sheet is provided for technical reference. The Safety Data Sheet (SDS) controls in all cases where guidance differs. Values reflect Alliance Chemical canonical data at time of generation; subsequent revisions are recorded in the Revision History above.