

TECHNICAL DATA SHEET

Hexane ACS Reagent Grade

ACS Reagent

CAS NUMBER

110-54-3

ALLIANCE CODE

hexane-acs-reagent-grade

GENERATED

2026-08-31

REVISION

1.3

REVIEWED

2026-06-18 · Andre Taki

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 %	99.5 %	Gas chromatography (GC)	ACS Reagent Chemicals
n-Hexane	45.0% min.	57.5 %	—	ACS Reagent Chemicals

TEST	SPECIFICATION	TYPICAL	METHOD	SOURCE
Residue After Evaporation	0.001% max.	0.0002 %	—	ACS Reagent Chemicals
Sulfur Compounds (as S)	0.005% max.	0.00002 %	—	ACS Reagent Chemicals
Thiophene	To Pass Test	Passes test	—	ACS Reagent Chemicals
Water Soluble Titratable Acid	0.0003 meq/g max.	0.00001 meq/g	—	ACS Reagent Chemicals
Substances Darkened by Sulfuric Acid	To Pass Test	Passes test	ACS monograph procedure (sulfuric acid shake test), visual comparison	Interpreted

Specification values are guaranteed limits. Typical values are representative of production lots and are not guaranteed. Lot-specific certificates of analysis ship with every order.

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 shown is the rolling-window mean from the sibling product's most recent lots. Grade selection drives downstream end-use — verify the sibling grade matches your specification before substitution.

PHYSICAL & CHEMICAL PROPERTIES

PROPERTY	VALUE	SOURCE
Appearance	Passes Test (clear, colorless liquid)	ACS Reagent Chemicals
Form	Liquid	Published reference
Color	10 max.	ACS Reagent Chemicals
Odor	Gasoline-like odor	Published reference
Specific Gravity (20 °C)	0.655 – 0.685	Interpreted
Density	0.659 at 68 °F (USCG, 1999) – Less dense than water; will float	Published reference
Boiling Point	62 – 70 C	Interpreted
Melting Point	–139 °F (NTP, 1992)	Published reference
Flash Point	–9.4 °F (NTP, 1992)	Published reference
Vapor Pressure	120 mmHg at 68 °F ; 180 mmHg at 77 °F (NTP, 1992)	Published reference
Solubility (water)	less than 1 mg/mL at 61.7 °F (NTP, 1992)	Published reference
Refractive Index (nD 20)	1.372 – 1.380	Interpreted

MATERIALS OF CONSTRUCTION

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	—	Aromatic solvents swell and dissolve HDPE.	Cole-Parmer Chemical Compatibility

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**

PACKING GROUP

II **Adjudicated**

HAZARD CLASS

3 **Adjudicated**

PROPER SHIPPING NAME

Hexanes **Adjudicated**

GHS / OSHA HAZCOM 2012

SIGNAL WORD

Danger **Adjudicated**

H-CODES (HAZARD STATEMENTS)

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

ECHA CLP Annex VI

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 CLP Annex VI

OCCUPATIONAL EXPOSURE LIMITS

OSHA PEL (29 CFR 1910.1000)

500 ppm TWA **OSHA 29 CFR 1910.1000**

ACGIH TLV

— **no canonical**

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: ECHA CLP Annex VI for harmonised classifications, NIOSH Pocket Guide for REL/IDLH, OSHA Z-Tables for PEL. Always verify against the latest regulatory text before shipment-critical decisions.

CATALOG EQUIVALENTS CROSS-REFERENCE VS MAJOR CHEMICAL SUPPLIERS

SIGMA-ALDRICH

SKU	GRADE	CONC.	MATCH	NOTES
139386	ACS Reagent	95%	Exact	ACS Reagent ≥95%
296090	ACS reagent	≥98.5%	Exact	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.

APPLICATION GUIDANCE

Hexane ACS Reagent Grade (ACS Reagent) is a nonpolar solvent used for hydrocarbon extraction, coatings, and degreasing.

- Coatings, paints, and adhesives
- Industrial degreasing
- Hydrocarbon extraction and recovery
- Rubber and polymer processing
- Cleaning of oil-based residues

Highly flammable and electrostatic-prone. Use grounded transfer equipment and inert gas blanketing where appropriate.

STORAGE & HANDLING

RECOMMENDED STORAGE

Cool, well-ventilated flammable-liquid storage. Tightly sealed containers. Segregate from oxidizers. Bond and ground bulk storage; consider inert gas blanketing for volatile solvents. Class-level guidance — not product-specific; the SDS controls.

INCOMPATIBILITIES

Strong oxidizers, halogens, nitric acid. Some grades react with rubber and certain plastics — verify gasket and hose compatibility. Class-level guidance — not product-specific; the SDS controls.

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.

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)

UN1208, Hexanes, 3, PG II

Sourced from 49 CFR 172.101. Confirm against shipping documents and carrier requirements before tender.

NMFC CLASS
70

PLACARD
Flammable Liquid

PACKING GROUP
PG II

REVISION HISTORY

Last reviewed 2026-06-18 by Andre Taki, DOT Hazmat Specialist.

VERSION	DATE	CHANGE	TRIGGER
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
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.