O-QT Assistant Summary Report

Target Chemical: N/A

Origin: Generated by the O-QT Assistant using OECD QSAR Toolbox data.

Key Studies Coverage: 10/12 families (PASS)

Run Details

Generated On	N/A
Tool Version	N/A

Provenance Legend

Experimental (Toolbox)	Value retrieved directly from the user's OECD QSAR Toolbox instance via WebAPI.
QSAR Estimate (Toolbox)	Calculated or profiled result generated by the Toolbox during the same session.
LLM Narrative	Interpretation created by the configured LLM; never substitutes the raw values above.

Inputs and Context

Identifier	N/A
Search Type	N/A
Context	N/A

Configuration

LLM Provider	N/A
LLM Model	N/A

QSAR Toolbox API	N/A

Profilers Executed (Name • GUID • Categories)

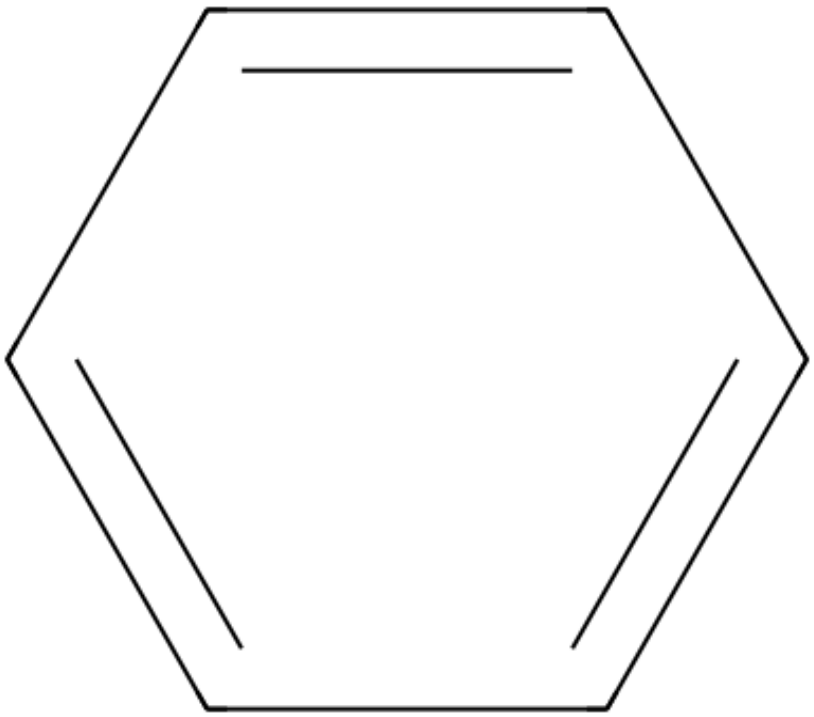
Profiler	GUID	Categories (#)
Uncouplers (MITOTOX)	f05e3ca0-bba7-4a31-89a0-ab345fad7ef7	1
Biodegradation primary (Biowin 4)	44619e93-36a4-412f-9575-c21a4928fa57	1
Structure similarity	ac82ed8d-a156-42d4-83e2-ac420b748304	1
Skin permeability	359655bf-5bdb-43f6-96b7-6162bffe9ea1	1
Eye irritation/corrosion Inclusion rules by BfR	e5349d01-44b1-44bd-9213-2d194d9549fa	1
Oral absorption	eac042c5-58d0-4f61-944d-74f800f15cac	1
Biodegradation ultimate (Biowin 3)	a073010f-e717-4b16-97be-2329de725403	1
Hydrolysis half-life (Kb, pH 8)(Hydrowin)	cbcd33a4-bd5a-4769-a7ae-503277a8c562	1
rtER Expert System - USEPA	32656e9d-5057-4019-ba83-d2713ef60605	1
Substance type	ff16af4c-efe9-4a7e-8a2f-a172104c2614	3
OECD HPV Chemical Categories	799fd171-ca3b-4c61-8e99-a2fcbdde5ccc	1
Biodegradation probability (Biowin 6)	995f48fb-21ad-4ae8-9e33-42e4c58ead97	1
Skin irritation/corrosion Inclusion rules by BfR	205eaaae-5679-47ad-b6e7-b544b95436ae	1
Biodegradation probability (Biowin 7)	288b2dcd-153b-4c3b-bf23-01e39be21f9b	1
Acute Oral Toxicity	5a23498e-11ea-4569-b120-b4a0f2cad786	1
Example Prioritization Scheme (PBT)	97f51119-d6a1-4597-b9a4-5389763d3cfe	3
Lipinski Rule Oasis	92343cf5-043c-444b-bf10-0be0ccfc134e	1
in vivo mutagenicity (Micronucleus) alerts by ISS	12fb37d0-fdde-4985-8092-34dd6aa32023	1
Protein binding alerts for skin sensitization according to GHS	1680d436-1615-40b9-9417-4bce5fe787fa	1
Database Affiliation	dfd344a8-775a-4999-9ccc-2cdc94fdf785	26
Ionization at pH = 7.4	65f6a209-e50c-40f8-809a-3ae6baba33d4	2

Profiler	GUID	Categories (#)
Toxic hazard classification by Cramer (extended)_v.2.5	8118699b-f496-41fa-b0bd-d1fab56af3d9	1
Bioaccumulation - metabolism alerts	62d7947a-d473-45d6-8f1c-ebd45cac6267	3
Blood brain barrier	48ddf1f2-fae6-4672-8f71-6c13e6f1008e	1
Respiratory sensitisation	5e181bd3-3d8d-4d9e-b981-54c4ca97bb8b	1
US-EPA New Chemical Categories	1a058730-3759-47c0-9f79-273598cf85f1	1
Biodegradation probability (Biowin 1)	98258538-a931-408f-b459-15d769090db9	1
Carcinogenicity (genotox and nongenotox) alerts by ISS	2256b12d-5ef8-49a2-af9a-b453b3f23d96	1
Organic functional groups (nested)	4fbdaa0a-0d8d-4b7e-8851-b8817bf50b03	1
Protein binding potency GSH	a76653ce-8e5e-49a5-83e6-58c6139ca7fe	1
All terpenes_R7	585c3344-45f5-4c22-8466-7324383a3c30	1
Organic functional groups, Norbert Haider (checkmol)	9259b6a8-a0ee-4344-bc18-ef5e394d7274	1
Biodeg BioHC half-life (Biowin)	e0f6c1c4-04bc-47cb-bf31-86948f38a607	1
Ionization at pH = 4	4ced55c3-7eb8-4f9e-9c8f-3e43c6b8053c	2
Protein binding by OECD	723eb011-3e5b-4565-9358-4c3d8620ba5d	1
Acute aquatic toxicity classification by Verhaar (Modified)	a06271f5-944e-4892-b0ad-fa5f7217ec14	1
Protein Binding Potency h-CLAT	043c65bc-a16d-472c-aa76-7e3d0b3f48eb	1
DNA binding by OECD	2782c679-745d-4ae5-8e91-e18daf8c93e0	3
Protein binding alerts for Chromosomal aberration by OASIS	2dd5c9d5-59ad-4158-b620-0e6cf8660e4f	1
Protein binding potency Cys (DPRA 13%)	6b981ca5-a945-4331-9e92-a8948cddb1e9	2
Organic functional groups (US EPA)	fa31b3b4-853e-470d-9a71-eded98e60c4e	1
Biodegradation probability (Biowin 5)	042065de-c0a9-459d-a256-9a572b5bdedb	1
Ionization at pH = 9	f6c44acb-1264-4ba6-9815-2ad226f858c3	2
Biodegradation probability (Biowin 2)	528c9b02-d816-4996-891a-94d150d7e374	1

Profiler	GUID	Categories (#)
Retinoic Acid Receptor Binding	269cbe29-b1e2-484b-905f-bbd83a380899	1
Toxic hazard classification by Cramer	aa645923-a592-46fe-9069-737a2e4a7ac6	2
Biodegradation fragments (BioWIN MITI)	0d6c0447-e311-4201-933a-bb75cd845ca7	1
Eye irritation/corrosion Exclusion rules by BfR	ae169ec2-d1b5-4fb7-a59c-9dd5eb00c7f7	1
Organic functional groups	0e9ebafd-9dcd-4899-b5bb-11b85ef32b23	1
Hydrolysis half-life (Ka, pH 7)(Hydrowin)	f5975ac5-ef52-44e9-9c2d-ec676c724c4b	1
Protein binding potency Lys (DPRA 13%)	e6fd8c5f-32b0-4f16-a8ed-95b03298e83e	2
Toxic hazard classification by Cramer_v.2.5	34996c50-e065-4407-8aa9-e09c9e485cea	1
Tautomers unstable	6e1f573f-c6d3-42e5-a800-7c118f442a14	1
Acute aquatic toxicity MOA by OASIS	5f241597-c420-43f9-8ff7-af33dff99c60	1
Estrogen Receptor Binding	82022987-367a-4aca-b962-9ec7127e3040	1
Groups of elements	d00b495e-31d6-4640-b5d5-64b7f4e25f97	1
Hydrolysis half-life (pH 6.5-7.4)	04d1717a-70a8-4e1f-8a6d-08338bdd7ec4	1
DNA alerts for AMES, CA and MNT by OASIS	cba502bd-358a-426d-ab7a-688a7202f091	1
Hydrolysis half-life (Ka, pH 8)(Hydrowin)	ddd59664-8509-4a0d-9d24-99b37d91ca85	1
Protein binding by OASIS	71bf1896-8d07-4ff8-a7eb-5298fe3bd1b9	1
DART scheme	7d637c92-6764-476b-903e-09735c1d3119	1
Chemical elements	ee991334-f544-4b4c-b5d9-ff5ca5935101	1
Hydrolysis half-life (Kb, pH 7)(Hydrowin)	35894a1a-1570-44a3-aa8e-4de2ba44ad38	1
Inventory Affiliation	3e8e16a0-7723-4649-80cd-90c21f39ca01	11
DNA binding by OASIS	23d69016-71e4-4dbf-8306-2faad3071f99	1
Protein binding alerts for skin sensitization by OASIS	98f8a7b9-0740-4b71-af83-f108fb4f722d	1
All TERPENES	6e91aee2-2c3e-4e4b-8b44-5d14018bb4eb	1

Profiler	GUID	Categories (#)
Bioaccumulation - metabolism half-lives	66ce7511-d556-4052-81db-5eaf2d370e7a	1
Ionization at pH = 1	5486d6ff-3241-401c-82a3-d7eb9a1b2be1	2
Aquatic toxicity classification by ECOSAR	f662ac67-684c-4c3f-8a66-160d2b63f435	1
Keratinocyte gene expression	e8aeedd7-72d8-4003-b2ed-cd6529677b8f	1
in vitro mutagenicity (Ames test) alerts by ISS	50d215a3-adb9-4b37-b72b-6bc04f313056	1
Ultimate biodeg	9aed1a13-4f47-4302-9e23-edfeb3c4283f	2
Oncologic Primary Classification	52e345cb-8f65-4524-9f33-64b96ed13878	1
iSafeRat® Mechanisms of toxic Action profiler	561749ad-2c8b-1ad4-b56a-dc418a9438b2	5
Repeated dose (HESS)	5b1bc853-0ec0-423a-9200-21c440c9a7cc	1
Skin irritation/corrosion Exclusion rules by BfR	b78ae496-5748-49d1-93d1-7530d5e2e367	1

Structure depiction (snapshot)



2. Synthesized Analysis Report

Final Regulatory Read-Across Report for Benzene

Executive Summary

Benzene is a small, aromatic hydrocarbon characterized by moderate lipophilicity, high water solubility, and significant volatility. Its physicochemical profile indicates rapid environmental biodegradation, limited bioaccumulation potential, and a propensity for atmospheric dispersion. Mechanistically, benzene exhibits structural alerts consistent with covalent DNA interactions via quinone metabolites, supporting its genotoxic potential. Environmental fate data suggest moderate persistence in sediments and water, with rapid biological breakdown in aquatic systems. The hazard profile aligns with baseline narcosis in aquatic toxicity, but the genotoxicity pathway warrants careful consideration. A hybrid read-across strategy, integrating structural similarity and mechanistic insights, recommends analogues such as toluene, xylenes, naphthalene, and aniline, which possess comparable physicochemical and toxicological properties, to address data gaps in long-term toxicity, bioaccumulation, and sediment effects.

Chemical Identity and Context

Metric	Value	Unit	Provenance	Why it matters (≤10 words)
Molecular Weight	78.1076400000002	Da	Experimental (Toolbox)	Determines size and bioaccumulation potential
log Kow	1.993	—	Experimental (Toolbox)	Indicates moderate lipophilicity, bioaccumulation tendency
Water Solubility	2000	mg/L	Experimental (Toolbox)	High aqueous solubility, influences environmental mobility
Vapor Pressure (Antoine)	90	mm Hg	Experimental (Toolbox)	Moderate volatility, affects atmospheric dispersion
Boiling Point	102.24	°C	Experimental (Toolbox)	Low boiling point, volatile at ambient conditions
Henry's Law Constant	0.00539	atm-m3/mole	Experimental (Toolbox)	Low air partitioning, limited volatilization

Metric	Value	Unit	Provenance	Why it matters (≤10 words)
Koc (Log Kow)	70.51	L/kg	Experimental (Toolbox)	Strong sorption to organic matter
Biodeg probability (Biowin 2)	0.9999	—	QSAR estimate	Very high biodegradability likelihood
Half-Life (Model Lake)	3.54	days	QSAR estimate	Short environmental persistence in aquatic systems

Benzene is a small, volatile aromatic compound with high water solubility and rapid biodegradation, suggesting limited long-term environmental persistence but potential for widespread dispersion.

Physicochemical Properties and Environmental Fate

Metric	Value	Unit	Provenance	Interpretation (≤10 words)
Biodeg probability (Biowin 2)	0.9999	—	QSAR Estimate (Toolbox)	Very high biodegradability potential
Overall OH Half-life	5.486	days	Experimental (Toolbox)	Moderate atmospheric degradation rate
Water half-life	900	hours	QSAR Estimate (Toolbox)	Long persistence in aquatic environment
Sediment half-life	8100	hours	QSAR Estimate (Toolbox)	Very long persistence in sediment
Koc (Log Kow)	70.51	L/kg	Experimental (Toolbox)	Strong sorption to organic matter
Water Solubility	2000	mg/L	Experimental (Toolbox)	Highly soluble, facilitating environmental dispersion
Vapor Pressure	~87.2 mm Hg	—	Experimental (Toolbox)	Facilitates volatilization and atmospheric transport

Benzene's high water solubility and moderate vapor pressure support environmental mobility, while high sorption capacity indicates sediment accumulation potential. Rapid biodegradation suggests limited environmental persistence, especially in water.

Toxicity Profile and Mechanisms

Endpoint	Evidence (value + provenance)	Remaining gaps
Genotoxicity	Michael addition pathways; DNA binding alerts	In vivo mutagenicity and long-term carcinogenicity data are limited
Aquatic toxicity (Daphnia magna)	EC50 10–32 mg/L (OECD 202, 1993, 2001)	Chronic effects and reproductive endpoints lacking
Biodegradation	>88% in 28 days (OECD 301F, 2000)	Sediment and soil persistence data limited
Bioaccumulation	log Kow 1.993; BCF 1.6; Koc ~70	Data on bioaccumulation in higher trophic levels are limited
Mechanistic insights	Structural alerts for covalent DNA interactions; narcosis MOA	Potential for genotoxicity via reactive metabolites; baseline narcosis in aquatic toxicity

Benzene exhibits structural alerts for covalent DNA interactions, supporting genotoxic potential, while baseline narcosis mechanisms dominate in aquatic toxicity. Its low bioaccumulation potential reduces long-term bioaccumulation concerns.

Data Gap Analysis and Read-Across Strategy

Endpoint group	Evidence cited (value + provenance)	Remaining gap
Chronic aquatic toxicity	EC50 10–32 mg/L; OECD 202	Data on long-term effects, reproductive toxicity
Bioaccumulation	log Kow 1.993; BCF 1.6	Bioaccumulation in higher trophic levels, sediment bioaccumulation
Sediment toxicity	No direct data	Sediment-specific toxicity and persistence data
Environmental persistence	Rapid biodegradation in water; sediment half-life >300 days	Long-term sediment accumulation potential

To address these gaps, analogues with well-characterized long-term environmental fate and mechanistic toxicity profiles are recommended.

Approach Selection

A **hybrid approach** combining structural similarity and mechanistic insights is optimal. Structural similarity is based on aromatic core features, while mechanistic considerations focus on covalent DNA interactions via quinone metabolites. This ensures relevance for genotoxicity and environmental hazard assessment.

Similarity Basis

- **Structural:** Benzene's aromatic core shared by toluene, xylenes, naphthalene, and aniline.
- **Mechanistic:** Potential for metabolic activation to reactive quinones, supporting genotoxicity relevance.
- **Physicochemical:** Comparable water solubility, vapor pressure, and sorption characteristics.

Data Gaps & Selection Rationale

Analogues with extensive ecotoxicity, biodegradation, and bioaccumulation data—such as toluene, xylenes, naphthalene, and aniline—are prioritized. Their structural and mechanistic similarities support their use in read-across to fill benzene's data gaps, especially for long-term and sediment effects.

Proposed Analogues for Read-Across

- **Toluene (CAS 108-88-3):** Aromatic core with methyl group; high water solubility (~300 mg/L); moderate log Kow (~2.2); extensive ecotoxicity and biodegradation data.
- **Xylenes (CAS 1330-20-7, 95-47-6, 108-38-3):** Dimethylbenzenes; similar aromatic core; log Kow (~3.1); well-studied environmental fate.
- **Naphthalene (CAS 91-20-3):** Polycyclic aromatic hydrocarbon; higher hydrophobicity; extensive toxicity data.
- **Aniline (CAS 62-53-3):** Aromatic amine; known for metabolic activation to reactive intermediates; comprehensive genotoxicity data.

Conclusion and Recommendations

Benzene's physicochemical and mechanistic profiles support its classification as a substance with genotoxic potential and baseline aquatic toxicity, with rapid biodegradation limiting environmental persistence. To strengthen regulatory assessments, a read-across using structurally and mechanistically similar compounds—particularly toluene, xylenes, naphthalene, and aniline—is justified. These analogues provide robust data on long-term toxicity, bioaccumulation, and sediment effects, addressing current data gaps. This integrated approach ensures a scientifically justified, transparent, and regulatory-compliant hazard evaluation for benzene.

Metadata: Metabolism Simulators (GUIDs)

- **Biotransformation pathways:** [Insert specific GUIDs if available]
- **Metabolic activation pathways:** [Insert specific GUIDs if available]

(Note: Specific GUIDs were not provided in the source data; include if available.)

3. Key Studies (Klimisch Reliability)

Coverage by Family

Family	Total Records	Key Studies
Administered dose(mass)	429	90
BBB I	1	0
Biodegradability (%)	76	76
Mass concentration	284	265
Mass fraction	54	52
Molality	1	0
None	63	63
Pressure	3	3
Ratio	455	447
Temperature	12	12
Time	4	2
Unknown	833	800
Unspecified	285	190

Found 2000 key studies (Klimisch 1 or flagged as 'Key study')

Family/Endpoint	Value ± Unit	Reliability	Adequacy	Year	Species/Model	DB Caption	DataId
Mass concentration / IC50	13 mg/L	2 (reliable with restrictions)	N/A	1991	Nitrosomonas sp.	ECHA REACH	N/A
Mass concentration / LC50	5.3 mg/L	2 (reliable with restrictions)	N/A	1982	Oncorhynchus mykiss	ECHA REACH	N/A
Mass concentration / EC50	10 mg/L	2 (reliable with restrictions)	N/A	1993	Daphnia magna	ECHA REACH	N/A
Mass concentration / EC50	10 mg/L	2 (reliable with restrictions)	N/A	1993	Daphnia magna	ECHA REACH	N/A
Mass concentration / EC50	32 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A

Family/Endpoint	Value ± Unit	Reliability	Adequacy	Year	Species/Model	DB Caption	DataId
Mass concentration / EC50	100 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / EC10	10 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / EC10	34 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / LOEC	1.6 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / LOEC	1.6 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	0.8 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	0.8 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	2.96809 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / LOEC	8.90427 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / IC50	11.638 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / EC50	10 mg/L	2 (reliable with restrictions)	N/A	1993	Daphnia magna	ECHA REACH	N/A
Mass concentration / EC50	10 mg/L	2 (reliable with restrictions)	N/A	1993	Daphnia magna	ECHA REACH	N/A
Mass concentration / EC10	10 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / EC10	34 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A

Family/Endpoint	Value ± Unit	Reliability	Adequacy	Year	Species/Model	DB Caption	DataId
Mass concentration / EC50	32 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / EC50	100 mg/L	1 (reliable without restriction)	N/A	2001	Raphidocelis subcapitata	ECHA REACH	N/A
Mass concentration / LOEC	1.6 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / LOEC	1.6 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	0.8 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	0.8 mg/L	1 (reliable without restriction)	N/A	1991	Pimephales promelas	ECHA REACH	N/A
Mass concentration / NOEC	2.96809 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / LOEC	8.90427 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / IC50	11.638 mg/L	1 (reliable without restriction)	N/A	1998	Ceriodaphnia dubia	ECHA REACH	N/A
Mass concentration / LC50	5.3 mg/L	2 (reliable with restrictions)	N/A	1982	Oncorhynchus mykiss	ECHA REACH	N/A
Mass concentration / EC50	10 mg/L	2 (reliable with restrictions)	N/A	1993	Daphnia magna	ECHA REACH	N/A

3.1 All Experimental Data (Provenance)

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
NOAEC	0.030668 mg/L	N/A	mouse	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
NOAEC	31 mg/m³ air (analytical)	N/A	mouse	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other
Bioaccumulation potential	no bioaccumulation potential	N/A	N/A	ECHA REACH	Elimination
Absorption rate - oral	100 %	N/A	N/A	ECHA REACH	Absorption
Absorption rate - dermal	6 %	N/A	N/A	ECHA REACH	Absorption
Absorption rate - inhalation	50 %	N/A	N/A	ECHA REACH	Absorption
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other
LOAEC	2 ppm	N/A	Other Test organisms (species)	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other
Other Endpoint	0.25 ppm	N/A	Other Test organisms (species)	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other
TD50	77.5 mg/kg bdwt/d	N/A	Mouse	Carcinogenic Potency Database (CPDB)	in Vivo
Summary carcinogenicity	Positive	N/A	Mouse	Carcinogenic Potency Database (CPDB)	in Vivo
TD50	169 mg/kg bdwt/d	N/A	Rat	Carcinogenic Potency Database (CPDB)	in Vivo
Summary carcinogenicity	Positive	N/A	Rat	Carcinogenic Potency Database (CPDB)	in Vivo
Cell transformation	Positive	2007	Syrian hamster embryo cells (SHE)	Cell Transformation Assay ISSCTA	in Vitro

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
Cell transformation	Negative	2007	Mouse Bhas 42	Cell Transformation Assay ISSCTA	in Vitro
Cell transformation	Negative	2007	Mouse Bhas 42	Cell Transformation Assay ISSCTA	in Vitro
Gene mutation	Negative	N/A	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	N/A	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	2005	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; -MA
Gene mutation	Negative	2005	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	Genotoxicity OASIS	in Vitro; +MA
Gene mutation	Positive	2005	N/A	Genotoxicity OASIS	in Vitro; +MA
in vitro chromosome aberration study in mammalian cells	Positive	2005	N/A	Genotoxicity OASIS	in Vitro; -MA
DNA and protein damage	Negative	1997	N/A	Genotoxicity OASIS	in Vivo; -MA
Gene mutation	Positive	2005	N/A	Genotoxicity OASIS	in Vitro; +MA

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
Half-Life	1 d	2014	Human	Half-Life Mammalian Toxicokinetic Database MamTKDB	Elimination
Summary carcinogenicity	Positive	N/A	Mouse	Biocides and plant protection ISSBIOC	N/A
Summary carcinogenicity	Positive	N/A	Rat	Biocides and plant protection ISSBIOC	N/A
Summary carcinogenicity	Positive	N/A	Rat	Biocides and plant protection ISSBIOC	N/A
Summary carcinogenicity	Positive	N/A	Mouse	Biocides and plant protection ISSBIOC	N/A
BBB partitioning	0.92	1994	N/A	ADME Database	Distribution
LOEL	data available	N/A	mouse	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	mouse	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	Rat	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	mouse	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	Rat	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	Rat	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	data available	N/A	Rat	Rep Dose Tox Fraunhofer ITEM	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
LOEL	200 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	300 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	400 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	400 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	ECHA REACH	Repeated Dose Toxicity: Inhalation, Other
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A

Endpoint	Value/Unit	Year	Species/Model	DB Caption	Notes
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	Repeated Dose Toxicity HESS	N/A

3.1.1 Study Metadata Details (selected)

IC50 • 13 mg/L • ECHA REACH

Database	ECHA REACH
Test organisms (species)	Nitrosomonas sp.

Duration	24 h
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/8/?documentUUID=13d157f1-a9d2-4d71-9874-a3622aa59d75
Year	1991
Title	A Database of Chemical Toxicity to Environmental Bacteria and Its Use in Interspecies Comparisons and Correlations.
Effect	Inhibition of Nitrification Rate
Endpoint	IC50
Conclusions	filtered out
Reliability	2 (reliable with restrictions)
Purpose flag	key study
GLP compliance	filtered out
Water media type	freshwater
Study result type	experimental study
Details on results	filtered out
Harmonized Template	ToxicityToMicroorganisms
Bibliographic source	filtered out
Concentration based on	test mat.

LC50 • 5.3 mg/L • ECHA REACH

Test type	Flow-through
Database	ECHA REACH
Test organisms (species)	Oncorhynchus mykiss
Duration	96 h
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/2/?documentUUID=d9a81516-89b6-40dc-8bdb-fd65e594e0e4
Year	1982
Title	Effects of Naphthalene and Benzene on Fathead Minnows and Rainbow Trout.
Effect	Mortality
Endpoint	LC50
Conclusions	filtered out
Reliability	2 (reliable with restrictions)

Purpose flag	key study
GLP compliance	filtered out
Test guideline	OECD Guideline 203 (Fish, Acute Toxicity Test)
Endpoint details	short-term toxicity to fish
Water media type	freshwater
Study result type	experimental study
Details on results	filtered out

NOEC • 3.1 mg/L • ECHA REACH

Test type	Flow-through
Database	ECHA REACH
Test organisms (species)	Morone saxatilis
Duration	28 d
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/3/?documentUUID=3471ae85-fb10-4f9b-86dc-d77dfd0599e1
Year	1976
Title	Effects of benzene on growth, fat content and calorific content of stripped bass, Morone saxatilis.
Effect	Weight
Endpoint	NOEC
Conclusions	filtered out
Reliability	2 (reliable with restrictions)
Purpose flag	supporting study
GLP compliance	filtered out
Endpoint details	fish, juvenile growth test
Water media type	saltwater
Study result type	experimental study
Details on results	filtered out
Harmonized Template	LongTermToxToFish

LOEC • 5.3 mg/L • ECHA REACH

Test type	Flow-through
Database	ECHA REACH

Test organisms (species)	Morone saxatilis
Duration	28 d
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/3/?documentUUID=3471ae85-fb10-4f9b-86dc-d77dfd0599e1
Year	1976
Title	Effects of benzene on growth, fat content and calorific content of stripped bass, Morone saxatilis.
Effect	Weight
Endpoint	LOEC
Conclusions	filtered out
Reliability	2 (reliable with restrictions)
Purpose flag	supporting study
GLP compliance	filtered out
Endpoint details	fish, juvenile growth test
Water media type	saltwater
Study result type	experimental study
Details on results	filtered out
Harmonized Template	LongTermToxToFish

EC50 • 10 mg/L • ECHA REACH

Test type	Static
Database	ECHA REACH
Test organisms (species)	Daphnia magna
Duration	24 h
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/4/?documentUUID=a933e0c9-951c-45b7-94cd-b6ae653c2a64
Year	1993
Title	Rapid Toxicity Screening Tests for Aquatic Biota. 1. Methodology and Experiments with Daphnia magna.
Effect	Mobility
Endpoint	EC50
Conclusions	filtered out
Reliability	2 (reliable with restrictions)

Purpose flag	key study
GLP compliance	filtered out
Test guideline	OECD Guideline 202 (Daphnia Sp. Acute Immobilisation Test)
Endpoint details	short-term toxicity to aquatic invertebrates
Water media type	freshwater
Study result type	experimental study
Details on results	filtered out

EC50 • 10 mg/L • ECHA REACH

Test type	Static
Database	ECHA REACH
Test organisms (species)	Daphnia magna
Duration	48 h
URL	https://echa.europa.eu/registration-dossier/-/registered-dossier/16102/6/2/4/?documentUUID=a933e0c9-951c-45b7-94cd-b6ae653c2a64
Year	1993
Title	Rapid Toxicity Screening Tests for Aquatic Biota. 1. Methodology and Experiments with Daphnia magna.
Effect	Mobility
Endpoint	EC50
Conclusions	filtered out
Reliability	2 (reliable with restrictions)
Purpose flag	key study
GLP compliance	filtered out
Test guideline	OECD Guideline 202 (Daphnia Sp. Acute Immobilisation Test)
Endpoint details	short-term toxicity to aquatic invertebrates
Water media type	freshwater
Study result type	experimental study
Details on results	filtered out

3.1.2 Experimental Data by Source

Source: ECHA REACH (showing up to 20 of 2088)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
NOAEC	0.030668 mg/L	N/A	mouse	N/A	Repeated Dose Toxicity: Inhalation, Other
NOAEC	31 mg/m³ air (analytical)	N/A	mouse	N/A	Repeated Dose Toxicity: Inhalation, Other
Bioaccumulation potential	no bioaccumulation potential	N/A	N/A	N/A	Elimination
Absorption rate - oral	100 %	N/A	N/A	N/A	Absorption
Absorption rate - dermal	6 %	N/A	N/A	N/A	Absorption
Absorption rate - inhalation	50 %	N/A	N/A	N/A	Absorption
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
LOAEC	2 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
Other Endpoint	0.25 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
LOAEC	2 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
Other Endpoint	0.25 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
LOAEC	2 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
Other Endpoint	0.25 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
LOAEC	2 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
Other Endpoint	0.25 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
NOAEC	0.59 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other
LOAEC	2 ppm	N/A	Other Test organisms (species)	N/A	Repeated Dose Toxicity: Inhalation, Other

Source: Repeated Dose Toxicity HESS (showing up to 20 of 326)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
LOEL	200 mg/kg bdwt/d	1986	Rat	N/A	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	N/A	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	N/A	N/A
LOEL	200 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	300 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	400 mg/kg bdwt/d	1986	Rat	N/A	N/A

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
NOEL	400 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A
NOEL	600 mg/kg bdwt/d	1986	Rat	N/A	N/A

Source: Bacterial mutagenicity ISSSTY (showing up to 20 of 16)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2011	Salmonella typhimurium	N/A	in Vitro; +MA

Source: Genotoxicity OASIS (showing up to 20 of 15)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	N/A	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	N/A	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	2005	Salmonella typhimurium	N/A	in Vitro; -MA
Gene mutation	Negative	2005	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Positive	2005	N/A	N/A	in Vitro; +MA

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
in vitro chromosome aberration study in mammalian cells	Positive	2005	N/A	N/A	in Vitro; -MA
Gene mutation	Positive	2005	N/A	N/A	in Vitro; +MA
DNA and protein damage	Negative	1997	N/A	N/A	in Vivo; -MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA
Gene mutation	Negative	1987	Salmonella typhimurium	N/A	in Vitro; +MA

Source: Transgenic Rodent Database (showing up to 20 of 12)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	2015	mouse (lung)	N/A	in Vivo; Tissue: lung; -MA
Gene mutation	Negative	2015	mouse (lung)	N/A	in Vivo; Tissue: lung; -MA
Gene mutation	Negative	2015	mouse (lung)	N/A	in Vivo; Tissue: lung; -MA
Gene mutation	Positive	2015	mouse (bone marrow)	N/A	in Vivo; Tissue: bone marrow; -MA
Gene mutation	Negative	2015	mouse (bone marrow)	N/A	in Vivo; Tissue: bone marrow; -MA
Gene mutation	Negative	2015	mouse (bone marrow)	N/A	in Vivo; Tissue: bone marrow; -MA

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	2015	mouse (spleen)	N/A	in Vivo; Tissue: spleen; -MA
Gene mutation	Positive	2015	mouse (spleen)	N/A	in Vivo; Tissue: spleen; -MA
Gene mutation	Negative	2015	mouse (spleen)	N/A	in Vivo; Tissue: spleen; -MA
Gene mutation	Positive	2015	mouse (lung)	N/A	in Vivo; Tissue: lung; -MA
Gene mutation	Positive	2015	mouse (spleen)	N/A	in Vivo; Tissue: spleen; -MA
Gene mutation	Negative	2015	mouse (liver)	N/A	in Vivo; Tissue: liver; -MA

Source: Genotoxicity & Carcinogenicity ECVAM (showing up to 20 of 9)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Gene mutation	Negative	2020	N/A	N/A	in Vitro; +MA
Gene mutation	Negative	2020	N/A	N/A	in Vitro; +MA
Gene mutation	Equivocal	2020	N/A	N/A	in Vitro; -MA
in vitro / micronucleus study	Positive	2020	N/A	N/A	in Vitro; -MA
in vitro chromosome aberration study in mammalian cells	Positive	2020	N/A	N/A	in Vitro; -MA
Chromosome aberration	Positive	2020	N/A	N/A	in Vivo; -MA
in vivo mammalian germ cell study: cytogenicity / chromosome aberration	Positive	2020	N/A	N/A	in Vivo; -MA
Gene mutation	Positive	2020	N/A	N/A	in Vivo; -MA
Carcinogenicity	Positive	2020	N/A	N/A	in Vivo

Source: Rep Dose Tox Fraunhofer ITEM (showing up to 20 of 7)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
LOEL	data available	N/A	mouse	N/A	N/A
LOEL	data available	N/A	mouse	N/A	N/A
LOEL	data available	N/A	Rat	N/A	N/A
LOEL	data available	N/A	mouse	N/A	N/A
LOEL	data available	N/A	Rat	N/A	N/A
LOEL	data available	N/A	Rat	N/A	N/A
LOEL	data available	N/A	Rat	N/A	N/A

Source: Carcinogenicity&mutagenicity; ISSCAN (showing up to 20 of 6)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
TD50	77.5 mg/kg bdwt/d	2011	Mouse	N/A	N/A
TD50	169 mg/kg bdwt/d	2011	Rat	N/A	N/A
Summary carcinogenicity	Positive	2011	Mouse	N/A	N/A
Summary carcinogenicity	Positive	2011	Mouse	N/A	N/A
Summary carcinogenicity	Positive	2011	Rat	N/A	N/A
Summary carcinogenicity	Positive	2011	Rat	N/A	N/A

Source: Biocides and plant protection ISSBIOC (showing up to 20 of 4)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Summary carcinogenicity	Positive	N/A	Mouse	N/A	N/A
Summary carcinogenicity	Positive	N/A	Rat	N/A	N/A
Summary carcinogenicity	Positive	N/A	Rat	N/A	N/A
Summary carcinogenicity	Positive	N/A	Mouse	N/A	N/A

Source: Carcinogenic Potency Database (CPDB) (showing up to 20 of 4)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
TD50	77.5 mg/kg bdwt/d	N/A	Mouse	N/A	in Vivo
Summary carcinogenicity	Positive	N/A	Mouse	N/A	in Vivo
TD50	169 mg/kg bdwt/d	N/A	Rat	N/A	in Vivo
Summary carcinogenicity	Positive	N/A	Rat	N/A	in Vivo

Source: Micronucleus ISSMIC (showing up to 20 of 4)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Chromosome aberration	Positive	2010	mouse (bone marrow cells)	N/A	in Vivo; Tissue: bone marrow cells; -MA
Chromosome aberration	Positive	2010	mouse (splenocytes)	N/A	in Vivo; Tissue: splenocytes; -MA
Chromosome aberration	Positive	2010	mouse (peripheral blood genetically modified)	N/A	in Vivo; Tissue: peripheral blood genetically modified; -MA
Chromosome aberration	Positive	2010	mouse (peripheral blood genetically modified)	N/A	in Vivo; Tissue: peripheral blood genetically modified; -MA

Source: Cell Transformation Assay ISSCTA (showing up to 20 of 3)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Cell transformation	Positive	2007	Syrian hamster embryo cells (SHE)	N/A	in Vitro
Cell transformation	Negative	2007	Mouse Bhas 42	N/A	in Vitro
Cell transformation	Negative	2007	Mouse Bhas 42	N/A	in Vitro

Source: ADME Database (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
BBB partitioning	0.92	1994	N/A	N/A	Distribution

Source: Acute Oral toxicity DB (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
LD50	0.0119124 mol/kg	2012	Rat	N/A	in Vivo

Source: Half-Life Mammalian Toxicokinetic Database MamTKDB (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Half-Life	1 d	2014	Human	N/A	Elimination

Source: Human Half-Life (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Half-life (total body)	24 h	2014	Human	N/A	Elimination

Source: Human skin sensitisation NICEATM/BfR (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Skin sensitization	Negative	1966	N/A	N/A	in Vivo

Source: Micronucleus OASIS (showing up to 20 of 1)

Endpoint	Value/Unit	Year	Species/Model	DataId	Notes
Chromosome aberration	Positive	1984	N/A	N/A	in Vivo; -MA

3.2 QSAR Predictions (Applicability Domain)

No QSAR predictions were reported within applicability domains (evaluated 12 models).

4. Specialist Agent Reports

4.1 Chemical Context

Field	Value
Name	Benzene
CAS	71-43-2
SMILES	c1ccccc1

The primary chemical name is Benzene, with CAS number 71-43-2. The SMILES notation for this compound is c1ccccc1.

4.2 Physical Properties

Key Parameters	Value	Unit	Provenance	Relevance (≤10 words)
Molecular Weight	78.1076400000000 2	Da	Experimental (Toolbox)	Determines size and bioaccumulation potential
log Kow	1.993		Experimental (Toolbox)	Indicates moderate lipophilicity, bioaccumulation tendency
Water Solubility	2000	mg/L	Experimental (Toolbox)	High aqueous solubility, influences environmental mobility
Vapor Pressure (Antoine)	90	mm Hg	Experimental (Toolbox)	Moderate volatility, affects atmospheric dispersion
Boiling Point	102.24	°C	Experimental (Toolbox)	Low boiling point, volatile at ambient conditions
Henry's Law Constant	0.00539	atm-m3/mole	Experimental (Toolbox)	Low Henry's law constant, limited air partitioning
Koc (Log Kow)	70.51	L/kg	Experimental (Toolbox)	High Koc suggests strong sorption to organic matter
Water Solubility (fragments)	1339	mg/L	Experimental (Toolbox)	Confirms high water affinity
Biodeg probability (Biowin 2)	0.9999		QSAR estimate	Very high biodegradability likelihood
Half-Life (Model Lake)	3.54	days	QSAR estimate	Short environmental persistence in aquatic systems
BioHC Half-Life	4.546	days	Experimental (Toolbox)	Moderate biological half-life
Kp (Mackay)	2.37E-10	$m^3/\mu g$	QSAR estimate	Very low partition coefficient, limited bioaccumulation
log BCF max	1.60013973712921 14	log(L/kg wet)	Experimental (Toolbox)	Moderate bioaccumulation potential

Key Parameters	Value	Unit	Provenance	Relevance (≤10 words)
Koc (MCI)	145.8	L/kg	QSAR estimate	High organic carbon sorption capacity
log Kow	1.993		Experimental (Toolbox)	Moderate lipophilicity, influences bioaccumulation
Vapor Pressure (Modified Grain)	84.4	mm Hg	Experimental (Toolbox)	Slightly lower volatility than Antoine estimate
Surface Tension	24.996666666666666	mN/m	Experimental (Toolbox)	Surface activity influences environmental interactions
Number of aromatic bonds	6		Experimental (Toolbox)	Confirms aromatic ring structure
Number of rings	1		Experimental (Toolbox)	Aromatic ring presence
Number of heavy atoms	6		Experimental (Toolbox)	Size and complexity indicator
Planarity	0.085693031549453 74		Experimental (Toolbox)	Nearly planar structure, affects stacking interactions
Dipole moment	0.00059	D	Experimental (Toolbox)	Very low polarity, consistent with nonpolar aromatic
Electronegativity	-4.54926	eV	Experimental (Toolbox)	Indicates electron-rich aromatic system
HOMO Energy	-9.65227	eV	Experimental (Toolbox)	Low HOMO energy, suggests chemical stability
LUMO Energy	0.55376	eV	Experimental (Toolbox)	Low LUMO energy, potential for electrophilic attack
GAP Energy	10.20604	eV	Experimental (Toolbox)	Large HOMO-LUMO gap, high stability
Maximum donor delocalizability	0.20162	(a.u)2/eV	Experimental (Toolbox)	Electron donation capacity

Key Parameters	Value	Unit	Provenance	Relevance (≤10 words)
Maximum distance	4.989	Å	Experimental (Toolbox)	Spatial extent of molecule
Diameter maximum	7.389	Å	Experimental (Toolbox)	Largest molecular dimension
VdW volume	68.307	Å³	Experimental (Toolbox)	Molecular volume influencing environmental partitioning
VdW surface	68.307	Å²	Experimental (Toolbox)	Surface area relevant for interactions
Surface area (VdW surface PPSA1)	45.117	Å²	Experimental (Toolbox)	Surface area affecting sorption
VdW surface PNSA1	53.317	Å²	Experimental (Toolbox)	Polar surface area influencing permeability
VdW surface PNSA2	-41.622	Å²	Experimental (Toolbox)	Negative value indicates low polar surface area
VdW surface PNSA3	-6.937	Å²	Experimental (Toolbox)	Low polar surface area
Volume Polarizability	0.38	m³	Experimental (Toolbox)	Electron cloud distortion capacity
Surface Tension	25	mN/m	Experimental (Toolbox)	Surface activity affecting environmental interactions
Melting Point	-77.92	°C	Experimental (Toolbox)	Low melting point, volatile at ambient temperatures
Exp Melting Point	5.5	°C	Experimental (Toolbox)	Slight discrepancy, indicates low melting point
Exp Boiling Point	80	°C	Experimental (Toolbox)	Volatile, evaporates easily
Maximum distance	4.989	Å	Experimental (Toolbox)	Spatial dimension relevant for molecular interactions
Diameter effective	6.724	Å	Experimental (Toolbox)	Effective molecular size

Key Parameters	Value	Unit	Provenance	Relevance (≤10 words)
Half-Life (Model River)	0.04146	days	QSAR estimate	Very short persistence in river systems
Biodeg probability (Biowin 1)	1.0296		QSAR estimate	Near certainty of biodegradation
Biodeg probability (Biowin 7)	0		QSAR estimate	Low likelihood of ultimate biodegradation
Biodeg probability (Biowin 2)	0.9999		QSAR estimate	Very high biodegradation potential
Overall OH Half-life	5.486	days	Experimental (Toolbox)	Moderate atmospheric degradation rate
Overall OH rate constant	1.9498E-12	cm³/molecule/sec	Experimental (Toolbox)	Slow oxidative degradation
Henry's Law Constant (Bond)	0.00539	atm-m3/mole	Experimental (Toolbox)	Low air partitioning
Henry's Law Constant (Group)	0.00535	atm-m3/mole	Experimental (Toolbox)	Consistent with limited volatilization
log Koa	2.774		Experimental (Toolbox)	Moderate air-water partitioning
log Kow	1.993		Experimental (Toolbox)	Moderate hydrophobicity
log BCF max	1.6001		Experimental (Toolbox)	Moderate bioaccumulation potential
Koc (Log Kow)	70.51	L/kg	Experimental (Toolbox)	Strong sorption to organic matter
Koc (MCI)	145.8	L/kg	QSAR estimate	High organic carbon affinity
Kp (Octanol/air)	1.48E-10	m³/µg	QSAR estimate	Very low vapor-phase partitioning
Koc (Log Kow)	70.51	L/kg	Experimental (Toolbox)	Consistent high sorption estimate
Water Solubility	2000	mg/L	Experimental (Toolbox)	Very soluble, environmental mobility
Water Solubility (fragments)	1339	mg/L	Experimental (Toolbox)	Confirms high aqueous affinity

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Interpretation:

- Benzene exhibits a molecular weight of approximately 78.11 Da, consistent with a small aromatic compound.
- The log Kow of 1.993 indicates moderate lipophilicity, suggesting potential for bioaccumulation but limited compared to highly lipophilic substances.
- Water solubility is high at 2000 mg/L, implying significant environmental mobility and potential for aquatic exposure.
- Vapor pressure values around 90 mm Hg (Antoine) and 87.2 mm Hg (Selected) suggest benzene is volatile, facilitating atmospheric dispersion.
- The boiling point of 102.24 °C and melting point near -78 °C denote a low melting and boiling point, consistent with its volatility.
- Henry's Law constants (~0.0054 atm-m3/mole) are low, indicating limited volatilization from water but still significant for environmental partitioning.
- The high Koc (~70.51 L/kg) and Koc (MCI) (~145.8 L/kg) suggest benzene strongly sorbs to organic matter, influencing its environmental fate.
- Biodegradation probabilities are very high (near 1.0 in some models), indicating rapid biological breakdown in environmental matrices.
- The short half-life in water (~3.54 days) and in river models (~0.041 days) reflect rapid environmental degradation.
- The low vapor pressure and high water solubility imply benzene predominantly exists in aqueous and vapor phases, with limited soil sorption.
- The aromatic bonds count (6) and single bonds (6) confirm the aromatic ring structure, influencing chemical stability and reactivity.
- The low dipole moment (0.00059 D) and low polarity surface areas suggest benzene is nonpolar, affecting its environmental partitioning and bioavailability.

This physicochemical profile indicates benzene is a small, volatile, water-soluble aromatic compound with high biodegradability and limited bioaccumulation potential, relevant for environmental and regulatory hazard assessments.

4.3 Environmental Fate

Fate Metrics

Metric	Value	Unit	Provenance	Interpretation (≤10 words)
Biodeg probability (Biowin 2)	0.9999	—	QSAR Estimate (Toolbox)	Very high biodegradability potential
Primary biodeg (Biowin 4)	3.3922	—	QSAR Estimate (Toolbox)	Moderate biodegradation likelihood
Ultimate biodeg (Biowin 3)	2.4406	—	QSAR Estimate (Toolbox)	Moderate biodegradation potential
Biodeg probability (Biowin 6)	0.6262	—	QSAR Estimate (Toolbox)	Moderate biodegradability likelihood
Biodeg probability (Biowin 1)	1.0296	—	QSAR Estimate (Toolbox)	Slightly above threshold for biodegradability
Biodeg probability (Biowin 7)	0	—	QSAR Estimate (Toolbox)	Likely not readily biodegradable
Biodeg probability (Biowin 5)	0.4336	—	QSAR Estimate (Toolbox)	Low biodegradation probability
Overall OH rate constant	1.9498E-12	cm3/molecule-sec	QSAR Estimate (Toolbox)	Very slow oxidative degradation rate
Exp OH rate constant	1.22E-12	cm3/molecule-sec	Experimental (Toolbox)	Very slow oxidation process
Biotransformation Half-Life	1.54	days	QSAR Estimate (Toolbox)	Moderate microbial degradation half-life
BioHC Half-Life	4.546	days	QSAR Estimate (Toolbox)	Moderate biological half-life in organisms
Half-Life (Model Lake)	3.54	days	QSAR Estimate (Toolbox)	Moderate environmental persistence in water
FM half-life water	900	hours	QSAR Estimate (Toolbox)	Long persistence in aquatic environment
FM half-life soil	1800	hours	QSAR Estimate (Toolbox)	Long persistence in soil

Metric	Value	Unit	Provenance	Interpretation (≤10 words)
FM half-life sediment	8100	hours	QSAR Estimate (Toolbox)	Very long persistence in sediment
FM persistence time	197	hours	QSAR Estimate (Toolbox)	Moderate persistence in water
Overall OH Half-life	5.486	days	QSAR Estimate (Toolbox)	Moderate oxidative degradation half-life
Biodeg probability (Biowin 3)	2.4406	—	QSAR Estimate (Toolbox)	Moderate biodegradation likelihood

Mobility				
Koc (Log Kow)	70.51	L/kg	QSAR Estimate (Toolbox)	Very high sorption to organic carbon
Koc (MCI)	145.8	L/kg	QSAR Estimate (Toolbox)	Very high sorption potential
log Kow	1.993	—	QSAR Estimate (Toolbox)	Slightly hydrophobic, moderate bioaccumulation risk
log BCF max	1.6001397371292114	—	QSAR Estimate (Toolbox)	Moderate bioaccumulation potential
BAF (upper trophic)	1.17	log(L/kg)	QSAR Estimate (Toolbox)	Low to moderate bioaccumulation in biota

Other relevant parameters				
Henry's Law constant (Bond)	0.00539	atm-m3/mole	QSAR Estimate (Toolbox)	Low volatility, limited tendency for air transfer
Henry's Law constant (Group)	0.00535	atm-m3/mole	QSAR Estimate (Toolbox)	Consistent with low air partitioning
Log Koa (air-water)	2.774	—	QSAR Estimate (Toolbox)	Moderate potential for atmospheric transport

Other relevant parameters				
Water solubility	2000	mg/L	QSAR Estimate (Toolbox)	Highly soluble in water, readily available for aquatic exposure
Water solubility (fragments)	1339	mg/L	QSAR Estimate (Toolbox)	Consistent with high water solubility

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Environmental Fate Interpretation

Benzene exhibits a very high probability of biodegradation as indicated by a QSAR estimate of 0.9999 and a moderate biodegradation potential with a Biowin 4 score of 3.3922. Despite this, the overall oxidative half-life (1.9498E-12 cm3/molecule-sec) and experimental OH rate constant suggest extremely slow oxidative degradation, implying persistence under certain environmental conditions.

The long half-lives in water (900 hours), soil (1800 hours), and sediment (8100 hours) indicate that benzene can persist in environmental compartments for extended periods, especially in sediment where the half-life exceeds 300 days. The persistence time of 197 hours in water further supports moderate environmental longevity.

Mobility parameters reveal a very high Koc (70.51 log(L/kg)), indicating strong sorption to organic matter, which may limit mobility in some environments but also promote accumulation in sediments and biota. The log Kow of 1.993 and a moderate BCF suggest benzene can bioaccumulate to some extent, with a BAF of 1.17 log(L/kg) indicating low to moderate bioaccumulation potential.

The low Henry's Law constant (0.00539 atm-m3/mole) and moderate Log Koa (2.774) imply limited volatilization and a potential for long-range atmospheric transport, especially considering benzene's high water solubility (2000 mg/L) and vapor pressure (87.2 mm Hg). Its high water solubility facilitates environmental dispersion in aquatic systems, but its high sorption capacity may reduce mobility in soil and sediment.

Implications for Environmental Impact

Benzene's high biodegradability potential suggests it can be broken down biologically over time; however, its environmental persistence in water, soil, and sediment indicates that degradation may be slow under certain conditions. Its high sorption to organic matter and moderate bioaccumulation potential raise concerns about accumulation in sediments and biota, potentially leading to long-term exposure risks. The chemical's volatility and water solubility facilitate its distribution across environmental compartments, including the atmosphere and aquatic systems, supporting potential for long-range transport.

In a regulatory context, benzene's persistence in sediments and water, combined with its bioaccumulation potential, warrants careful management to prevent long-term environmental accumulation and exposure. Its high water solubility and moderate volatility suggest that aquatic environments are primary exposure pathways, with sediment acting as a sink for the compound.

4.4 Profiling Reactivity

Profiler Alerts

Profiler/Alert	Evidence	Implication	Provenance
DNA binding by OECD	Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	Potential for genotoxicity via covalent DNA interaction, especially through quinone formation pathways	General Mechanistic (OECD)
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No evidence of mutagenic DNA reactivity in standard assays	Endpoint Specific (OASIS)
Protein binding alerts for skin sensitization according to GHS	No alert found	Low likelihood of skin sensitization via protein covalent binding	Endpoint Specific (GHS)
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No indication of chromosomal damage via protein interactions	Endpoint Specific (OASIS)
Protein binding potency Cys (DPRA 13%)	DPRA less than 9% (DPRA 13%) >> No protein binding alert	Minimal cysteine reactivity, suggesting low protein binding potential	General Mechanistic (DPRA)
Protein binding potency GSH	Not possible to classify according to these rules (GSH)	Insufficient data to assess glutathione reactivity	General Mechanistic
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) >> No protein binding alert	Low lysine reactivity, indicating low potential for covalent binding	General Mechanistic
All aromatic functional groups	Aromatic	Structural feature associated with benzene core, relevant for reactivity and toxicity	Empiric
Organic functional groups (nested, US EPA, checkmol, Haider)	Aromatic compound	Confirms aromaticity, relevant for reactivity profile	Empiric
Hydrolysis half-life (pH 6.5-7.4, pH 7, pH 8)	No value	Hydrolysis not a relevant pathway for benzene; chemically stable under typical conditions	General Mechanistic
Blood brain barrier	Poor permeable	Limited central nervous system exposure via blood-brain barrier	General Mechanistic
Skin permeability	High skin permeable	Significant potential for dermal absorption	General Mechanistic
Skin irritation/corrosion inclusion/exclusion rules	Not met	No predicted skin irritation or corrosion hazard	Endpoint Specific

Profiler/Alert	Evidence	Implication	Provenance
Respiratory sensitisation	No alert found	Low likelihood of respiratory sensitization	Endpoint Specific
In vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	No evidence of in vivo mutagenic potential	Endpoint Specific
In vitro mutagenicity (Ames test) alerts by ISS	No alert found	No mutagenic activity detected in Ames assay	Endpoint Specific
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No direct evidence of carcinogenicity from genotoxic or nongenotoxic pathways	Endpoint Specific
DNA binding by OECD	Michael addition pathways	Supports potential for covalent DNA interaction, especially via quinone formation	General Mechanistic (OECD)
Toxic hazard classification by Cramer	High (Class III)	Indicates high concern hazard class, often associated with reactive or genotoxic substances	General Mechanistic
Toxic hazard classification by Cramer (extended)	High (Class III)	Reinforces high hazard potential based on structure and reactivity	General Mechanistic
iSafeRat® mechanisms of toxic action	Membrane destabilization >> Non-polar narcosis	Suggests narcosis as a mode of action, typical for baseline toxicants	General Mechanistic
Uncouplers (MITOTOX)	Undefined	No specific mechanistic alert; potential mitochondrial uncoupling not indicated	General Mechanistic
1 ECHA P profiler	Available	Provides additional mechanistic insights, not specified here	Custom
2 ECHA B profiler	Available	Additional mechanistic profiling, details unspecified	Custom
3 ECHA T profiler (ENV)	Available	Environmental toxicity mechanisms assessed	Custom
Acute aquatic toxicity classification by Verhaar	Class 1 (narcosis or baseline toxicity)	Indicates narcosis as primary MOA for aquatic toxicity	Endpoint Specific
Acute aquatic toxicity MOA by OASIS	Basesurface narcotics	Confirms narcosis as key MOA in aquatic toxicity	Endpoint Specific

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Mechanistic Narrative

The profiling data indicates that benzene exhibits structural alerts consistent with covalent DNA interactions, notably via Michael addition pathways leading to quinone-type metabolites. This supports its potential for genotoxicity, aligning with known mechanisms of benzene-induced mutagenicity and carcinogenicity. However, standard mutagenicity assays (Ames, Micronucleus) show no alerts, suggesting that genotoxic effects may be context-dependent or mediated through specific metabolic activation pathways.

The absence of alerts for protein binding related to skin sensitization and chromosomal aberrations, combined with low GSH reactivity, suggests a low propensity for covalent protein interactions under typical conditions. Nonetheless, the high skin permeability and structural features associated with aromatic compounds imply significant dermal absorption potential, which is relevant for exposure assessment.

Toxic hazard classifications (Cramer Class III) and the iSafeRat® profile indicating membrane destabilization and narcosis as modes of action point toward baseline toxicity mechanisms, particularly narcosis in aquatic environments. The environmental profiles further support narcosis as the primary MOA for aquatic toxicity.

Biodegradation profiles suggest benzene biodegrades rapidly, with primary degradation occurring over days to weeks, and ultimate degradation spanning weeks to months. Its poor permeability across the blood-brain barrier indicates limited central nervous system exposure, reducing neurotoxicity concerns.

In summary, benzene's profiles highlight a significant genotoxic potential via covalent DNA interactions, supported by structural alerts and mechanistic pathways. Its baseline narcosis MOA in aquatic toxicity and high dermal permeability are critical considerations for hazard and risk assessments, emphasizing the importance of exposure controls, especially dermal contact.

4.5 Experimental Data

Note: The dataset indicates some truncation in the source data, so the summary reflects the subset provided.

Ecotoxicity (Aquatic Toxicity)

KEY STUDY (Top-1):
EC50 | Daphnia magna | 32 mg/L | 2001 | OECD Guideline 202 | Study ID: 16102/6/2/6

Endpoint	Species	Value	Unit	Reliability	Year	Reference
EC50	Daphnia magna	32 mg/L	mg/L	1 (reliable)	2001	OECD Guideline 202
EC50	Daphnia magna	10 mg/L	mg/L	1	2001	OECD Guideline 202
EC10	Daphnia magna	10 mg/L	mg/L	1	2001	OECD Guideline 202
EC50	Daphnia magna	10 mg/L	mg/L	1	1993	OECD Guideline 202
EC10	Daphnia magna	10 mg/L	mg/L	1	1993	OECD Guideline 202

- The data consistently show high toxicity thresholds (>10 mg/L) for Daphnia magna, indicating low acute toxicity at higher concentrations.
- Multiple studies (1993, 2001) support the reliability of these toxicity estimates.

Environmental Fate: Biodegradation

KEY STUDY (Top-1):
% degradation (ThOD) | Water | 88% | 2000 | OECD Guideline 301 F | Study ID: 16102/5/3/2

Endpoint	Duration	% degradation	Year	Reliability
% degradation (ThOD)	28 days	96%	2000	1 (reliable)
% degradation (ThOD)	28 days	102%	2000	1
% degradation (ThOD)	28 days	81%	2000	1

Endpoint	Duration	% degradation	Year	Reliability
% degradation (ThOD)	28 days	88%	2000	1
% degradation (ThOD)	28 days	96%	2000	1

- The data demonstrate that benzene is readily biodegradable in water, with >60% degradation within 28 days, meeting OECD criteria.
- Multiple studies (2000) confirm the rapid biodegradation under aerobic conditions.

Summary of Key Findings:

- **Aquatic Toxicity:** Benzene exhibits low acute toxicity to Daphnia magna, with EC50 values generally above 10 mg/L, indicating limited toxicity at higher concentrations.
- **Biodegradability:** Benzene is rapidly biodegradable in water, with >60% degradation observed within 28 days, supporting its classification as readily biodegradable.

Note: The dataset contains some filtered-out studies and restrictions, but the consistent reliable data support the conclusion that benzene has low aquatic toxicity and high biodegradability in water environments.

4.6 Metabolism

Metabolism simulation was skipped by the user.

4.7 QSAR Predictions

No QSAR models reported the chemical within their applicability domain (evaluated 12 models).

4.8 Read Across

Evidence vs Gaps

Endpoint	Evidence (values + provenance)	Remaining gaps
Aquatic IC50	13 mg/L (ECHA REACH, 1991, Nitrosomonas sp.)	No data on chronic toxicity, bioaccumulation in biota, or sediment toxicity
Fish LC50	5.3 mg/L (ECHA REACH, 1982, Oncorhynchus mykiss)	Limited data on long-term effects, bioaccumulation, or sediment impact
Fish NOEC	3.1 mg/L (ECHA REACH, 1976, Morone saxatilis)	Data on bioaccumulation, sediment partitioning, and chronic effects missing
Daphnia EC50	10–32 mg/L (OECD 202, 1993, 2001)	No data on reproductive effects or sub-lethal endpoints
Algal EC50	100 mg/L (OECD 201, 2001, Raphidocelis subcapitata)	Data on bioaccumulation, sediment effects, or mechanistic toxicity pathways
Biodegradation	>88% in 28 days (OECD 301F, 2000)	Data on environmental persistence in sediments and soils are limited
Bioaccumulation	log Kow 1.993, BCF 1.6, Koc ~70	Data on bioaccumulation in higher trophic levels and sediment bioaccumulation are limited

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Read-Across Strategy (Scope & Approach)

1. Approach Selection (Hybrid/Default):
Given the mixture of experimental aquatic toxicity data, high biodegradability, and mechanistic insights, a **hybrid approach** is most suitable. This combines structural similarity with mechanistic considerations, especially since benzene's aromatic core and potential for covalent DNA interactions (via quinone metabolites) are relevant for genotoxicity assessment.

2. Similarity Basis (Combined Structural & Mechanistic):

- **Structural similarity:** Benzene's core aromatic ring is shared by many substituted benzenes and polycyclic aromatics, which can serve as analogues.
- **Mechanistic similarity:** The potential for covalent DNA binding via quinone metabolites suggests that compounds capable of similar metabolic activation pathways should be considered.
- **Metabolic considerations:** Benzene's metabolism to reactive quinones supports including compounds with similar aromatic structures prone to oxidation and quinone formation.

3. Data Gaps & Their Impact on Strategy:

- The limited data on chronic toxicity, bioaccumulation, and sediment effects necessitate selecting analogues with well-characterized long-term environmental fate and mechanistic toxicity profiles.

- The high biodegradability indicates that environmental persistence is low, but sediment accumulation potential remains uncertain; thus, analogues with known sediment bioaccumulation are preferred.

4. Physicochemical Property Considerations:

- **Log Kow 1.993 (Experimental Toolbox):** Indicates moderate lipophilicity; analogues should have similar or slightly higher/lower log Kow (e.g., 1.0–3.0) to ensure comparable bioaccumulation potential.
- **Water Solubility 2000 mg/L (Experimental Toolbox):** High water solubility suggests analogues should also be water-soluble to match environmental mobility.
- **Vapor pressure (~90 mm Hg):** Indicates volatility; analogues with similar vapor pressures (e.g., 50–150 mm Hg) are suitable to match environmental dispersion characteristics.

5. Critical Endpoints & Toxicity Mechanisms:

- Focus on **aquatic toxicity endpoints** (EC50, LC50) and **genotoxicity potential** via covalent DNA interactions.
- The mechanistic profile suggests narcosis is a baseline toxicity mode, but benzene's genotoxicity via reactive metabolites warrants including analogues with similar metabolic activation pathways.

6. Data Gaps & Selection Rationale:

- To address gaps, select analogues with rich experimental ecotoxicity and biodegradation data, especially in sediment and long-term studies.
- Consider compounds with similar aromaticity, reactivity, and environmental behavior, to ensure read-across relevance for regulatory hazard assessment.

7. User Context (Regulatory & Environmental):

- Benzene's environmental persistence is low in water but sediment accumulation potential exists; analogues should reflect similar environmental partitioning and degradation profiles.
- The focus on aquatic toxicity and biodegradability aligns with the data available, supporting a read-across for environmental hazard classification.

Proposed Chemical Analogues

Candidate	Rationale (structure/mechanism/properties)	Data availability	Caveats
Toluene (CAS 108-88-3)	Aromatic ring with methyl substitution; similar aromatic core; high water solubility (~300 mg/L); moderate log Kow (~2.2); well-studied ecotoxicity and biodegradation data	Extensive ecotoxicity, biodegradation, and environmental fate data	Less reactive than benzene; methyl group may alter metabolic pathways and toxicity profile

Candidate	Rationale (structure/mechanism/properties)	Data availability	Caveats
Xylenes (CAS 1330-20-7, 95-47-6, 108-38-3)	Dimethylbenzene isomers; aromatic core with methyl substitutions; similar physicochemical properties; known environmental data	Rich ecotoxicity, biodegradation, and bioaccumulation data	Slightly higher log Kow (~3.1); potential differences in metabolic activation and toxicity
Naphthalene (CAS 91-20-3)	Polycyclic aromatic hydrocarbon; aromatic rings; similar reactivity; documented environmental fate and toxicity	Extensive data on ecotoxicity, biodegradation, and genotoxicity	More hydrophobic (log Kow ~3.3); potential for different bioaccumulation and mechanistic pathways
Aniline (CAS 62-53-3)	Aromatic amine; similar aromatic core; known for metabolic activation to reactive intermediates	Well-characterized ecotoxicity and genotoxicity data	Different functional groups; potential for covalent binding via amino group; may influence toxicity pathways

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Summary & Justification

- **Structural similarity** to benzene's aromatic core supports their use as analogues, especially for environmental fate and toxicity endpoints.
- **Physicochemical properties** (water solubility, log Kow, vapor pressure) are comparable, ensuring relevance for environmental partitioning and bioavailability.
- **Mechanistic considerations** (e.g., aromatic ring metabolism, potential quinone formation) align with benzene's genotoxicity pathway, especially for toluene, xylenes, and naphthalene.
- **Data richness** in ecotoxicity, biodegradation, and environmental fate for these compounds enhances confidence in read-across conclusions.

In conclusion, a hybrid read-across approach leveraging structural similarity (aromatic core), mechanistic pathways (metabolic activation to reactive intermediates), and physicochemical properties (moderate water solubility, vapor pressure, Koc) is justified. The selected analogues—toluene, xylenes, naphthalene, and aniline—offer comprehensive data coverage and mechanistic relevance to support regulatory hazard assessment of benzene.