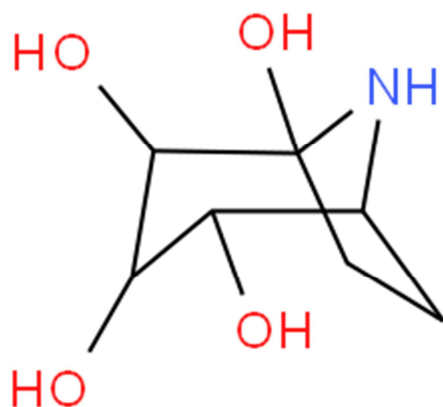


(Q)SAR predicted profile

Structure (as used for QSAR prediction):



SMILES (used for QSAR prediction): C12(O)C(O)C(O)C(O)C(CC1)N2

ID

EC Number (pre-registration)		EC Number (registration)	
Registry Number	178231-95-3	PubChem CID	
Chemical Name			
Molecular Formula	C7 H13 N1 O4	Molecular weight (g/mole)	175.19

Genotoxicity

Ashby Structural Alerts for DNA Reactivity

	Battery	CASE Ultra	Leadscope	SciQSAR
Ashby Structural Alerts	NEG_OUT	INC_OUT	INC_OUT	NEG_IN

Bacterial Reverse Mutation Test (Ames test)

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Ames test in <i>S. typhimurium</i> (<i>in vitro</i>)		NEG_IN	NEG_IN	NEG_IN	NEG_IN

Other *in vitro* Genotoxicity Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Chromosome Aberrations in Chinese Hamster Ovary (CHO) Cells	NA	NEG_IN	INC_OUT	NEG_IN	NEG_IN
Chromosome Aberrations in Chinese Hamster Lung (CHL) Cells		NEG_OUT	NEG_OUT	NEG_IN	INC_OUT
Mutations in Thymidine Kinase Locus in Mouse Lymphoma Cells		NEG_IN	INC_OUT	NEG_IN	NEG_IN
Mutations in HGPRT Locus in Chinese Hamster Ovary (CHO) Cells		NEG_IN	INC_OUT	NEG_IN	NEG_IN
Unscheduled DNA Synthesis (UDS) in Rat Hepatocytes		POS_OUT	INC_OUT	POS_IN	POS_OUT
Syrian Hamster Embryo (SHE) Cell Transformation		NEG_IN	INC_OUT	NEG_IN	NEG_IN

HGPRT: Hypoxanthine-guanine phosphoribosyltransferase

In vivo Genotoxicity Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Sex-Linked Recessive Lethal (SLRL) Test in <i>Drosophila m.</i>		INC_OUT	INC_OUT	POS_IN	NEG_IN
Micronucleus Test in Mouse Erythrocytes		NEG_IN	INC_OUT	NEG_IN	NEG_IN
Dominant Lethal Mutations in Rodents		NEG_IN	INC_OUT	NEG_IN	NEG_IN
Sister Chromatid Exchange in Mouse Bone Marrow Cells		NEG_OUT	INC_OUT	NEG_OUT	NEG_IN
Comet Assay in Mouse		NEG_IN	INC_OUT	NEG_IN	NEG_IN

Abbreviations

INC: inconclusive. A definite call within the defined applicability domain could not be made.

NEG: negative

POS: positive

IN: inside applicability domain

OUT: outside applicability domain

Exp: Experimental values, from EpiSuite experimental databases or DK DTU QSAR models training sets.

NA: Not applicable, because training set data cannot be released for commercial models.

Important notes

This is an automatically generated report from the Danish (Q)SAR Database, <http://qsar.food.dtu.dk>.

For predictions from CASE Ultra, Leadscope, SciQSAR as well as the Acute toxicity in rodent from ACDLabs information on the software versions can be found in the QMRFs. For the other predicted properties the software versions are:

EPI MPBPWIN v1.43

EPI HENRYWIN v3.20

EPI WSKOW v1.42

EPI WATERNT v1.01

EPI KOAWIN v1.10

EPI AEROWIN v1.00

EPI KOCWIN v2.00

EPI Level III Fugacity Model (EPI Suite v4.11)

EPI STPWIN (EPI Suite v4.11)

EPI AOPWIN v1.92

EPI BIOWIN v4.10

EPI BCFBAF v3.01

EPI ECOSAR v1.11

EPI DERMWIN v2.02

ACD/ ToxSuite 2.95.1 Ionization\pKa

ACD/ ToxSuite 2.95.1 Ionization\ LogD

ACD/ ToxSuite 2.95.1

It is recommended to run the latest version of the EPI Suite Programs in preference of the predictions given in this document when these endpoints are of importance and new versions have been released from the United States Environmental Protection Agency in comparisons. EPI Suite can be downloaded from the US EPA homepage: <http://www.epa.gov/oppt/exposure/pubs/episuitedi.htm>

For further information on the applied systems, see the following homepages:

CASE Ultra: <http://www.multicase.com/case-ultra>

Leadscope: <http://www.leadscope.com/>

SciQSAR: <http://lhasa-llc.com/>

ToxSuite: <http://www.acdlabs.com/>

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All access to the database should happen through the provided client-side software and without any use of automated workflow or scripting.

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