ProtoICH

EXPERT RULE-BASED PREDICTION DOSSIER

www.protoqsar.com

Centro Europeo de Empresas Innovadoras (CEEI)
Parque Tecnológico de Valencia
Avda. Benjamin Franklin 12
46980 Paterna (Valencia, Spain)

info@protoqsar.com

+34 962 021 811

ProtoQSAR
Chemoinformatics and modeling solutions to optimize your chemicals

1. Substance

1.1. CAS:

109-66-0

1.2. EC number:

203-692-4

1.3. Chemical name:

Pentane

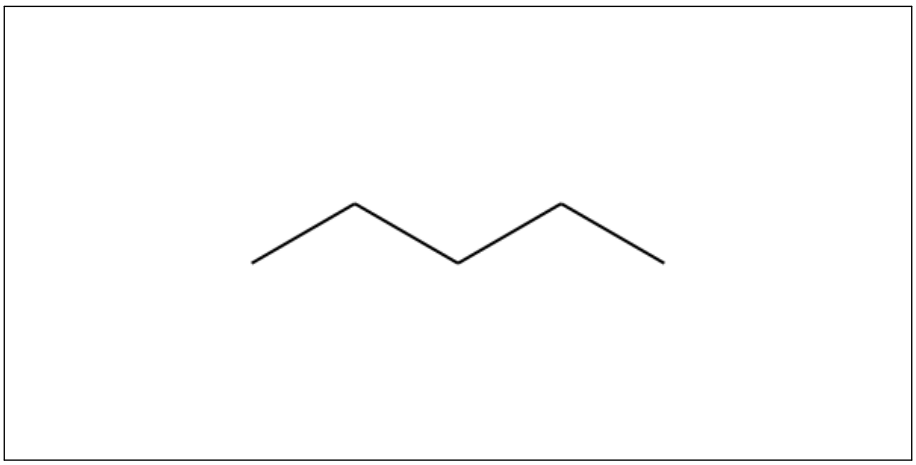
1.4. Structural formula:

C5H12

1.5. SMILES:

CCCCC

1.6. Structural representation:



2. General information

2.1. Date of Rule-based report:

21-Mar-2022

2.2. Report authorship and contact details:

- ***Authorship:*** ProtoQSAR
- ***Address:*** CEEI-Valencia Benjamin Franklin, 12.46980 Paterna
- ***Phone:*** +34 962 021 811
- ***Email:*** info@protoqsar.com

3. Prediction

3.1. Endpoint:

- ***Endpoint:*** Mutagenicity (Ames test)

3.2. Algorithm:

- ***Software name:*** ProtoICH software from ProtoQSAR has been used to perform the prediction.
- ***Software version:*** v 1.0
- ***Predicted value:*** . There are NO alerts for Mutagenicity (Ames test) endpoint
- ***Input for prediction:*** SMILES structure of point 1.5
- ***Rules-based results:***

ALERT	RESULT
SA1.-Acyl halides?	NO ALERT
SA2.-Alkyl (C<5) or benzyl ester of sulphonic or phosphonic acid?	NO ALERT
SA3.-N-methylol derivatives?	NO ALERT
SA4.-Monohaloalkene?	NO ALERT
SA5.-S or N mustard?	NO ALERT
SA6.-Propiolactones and propiosultones?	NO ALERT
SA7.-Epoxides and aziridines?	NO ALERT
SA8.-Aliphatic halogens?	NO ALERT
SA9.-Alkyl nitrite?	NO ALERT
SA10.-a,b unsaturated carbonyls?	NO ALERT
SA11.-Simple aldehyde?	NO ALERT
SA12.-Quinones?	NO ALERT
SA13.-Hydrazine?	NO ALERT
SA14.-Aliphatic azo and azoxy?	NO ALERT
SA15.-Isocyanate and isothiocyanate groups?	NO ALERT
SA16.-Alkyl carbamate and thiocarbamate?	NO ALERT
SA18.-Polycyclic Aromatic Hydrocarbons?	NO ALERT
SA19.-Heterocyclic Polycyclic Aromatic Hydrocarbons?	NO ALERT
SA21.-Alkyl and aryl N-nitroso groups?	NO ALERT
SA22.-Azide and triazene groups?	NO ALERT
SA23.-Aliphatic N-nitro?	NO ALERT
SA24.-a,b unsaturated alkoxy?	NO ALERT
SA25.-Aromatic nitroso group?	NO ALERT
SA26.-Aromatic ring N-oxide?	NO ALERT
SA27.-Nitro aromatic?	NO ALERT
SA28.-Primary aromatic amine, hydroxyl amine and its derived esters?	NO ALERT

SA28bis.-Aromatic mono- and dialkylamine?	NO ALERT
SA28ter.-Aromatic N-acyl amine?	NO ALERT
SA29.-Aromatic diazo with sulphonic groups?	NO ALERT
SA30.-Coumarins and Furocoumarins?	NO ALERT
SA37.-Pyrrolizidine Alkaloids?	NO ALERT
SA38.-Alkenylbenzenes?	NO ALERT
SA39.-Steroidal estrogens?	NO ALERT
SAaNNa.-Aromatic diazo?	NO ALERT
SAarNCH2.-Derived aromatic amines?	NO ALERT
QSA57_Ames.-DNA Intercalating Agents with a basic side chain?	NO ALERT
QSA58_Ames.-Haloalkene cysteine S-conjugates?	NO ALERT
QSA59_Ames.-Xanthones, Thioxanthones, Acridones?	NO ALERT
QSA60_Ames.-Flavonoids?	NO ALERT
QSA61_Ames.-Alkyl hydroperoxides?	NO ALERT
QSA62_Ames.-N-acyloxy-N -alkoxybenzamides?	NO ALERT
QSA63_Ames.-N-aryl-N-acetoxyacetamides?	NO ALERT
QSA64_Ames.-Hydroxamic acid derivatives?	NO ALERT
QSA65_Ames.-Halofuranones?	NO ALERT

4. Conclusions

4.1. Conclusion:

The ProtoQSAR rule-based model has been used for the prediction of the Mutagenicity (Ames test) endpoint for CCCCC. There are NO alerts for Mutagenicity (Ames test) endpoint.