

Substance Details Report

January 9, 2017

Core Metadata

Substance Type	Chemical Substance	Internal Tracking Number	52225
EPA Registry Name	5-Methyl-3-heptanone	Substance Status	Approved
EPA Registry Name List	Chemical Identification		
Systematic Name	3-Heptanone, 5-methyl-		
Systematic Name List	Chemical Abstracts Index Name		
Preferred Acronym			
CAS Number	541-85-5		
EPA Identification Number			
TSN Number			
Kingdom			
ICTVDB			
Molecular Formula	C8H16O		
Molecular Weight	128.21		
Comment/Description			

Definition

Classifications

Associated Identifiers

Former CAS Numbers

57968-70-4

Incorrect CAS Numbers

106-68-3

108-68-3

Structure

Notation

CCC(=O)CC(C)CC

Notation Type

SMILES

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Synonym

Below are the EPA applications/systems, statues/regulations, or other sources that track or regulate this substance. This table shows how each list refers to the substance.

Statutes/Regulations

Statutes/Regulations	Synonym	Synonym Quality	Effective Date	End Date
2016 CDR TSCA Inv	5-Methyl-3-heptanone	Valid		
TSCA Inv	3-Heptanone, 5-methyl-	Valid		

EPA Applications/Systems

EPA Application/System	Synonym	Synonym Quality	Effective Date	End Date
2012 CDR	3-Heptanone, 5-methyl-	Valid		
CERCLIS3	Ethyl sec-amyl ketone	Valid		
ECOTOX	5-Methyl-3-heptanone	Valid		
ERNS	5-Methyl-3-heptanone	Valid		
ICIS-Air	5-Methyl-3-heptanone	Valid	09/20/2013	
TSCA Inv Syms	5-Methyl-3-heptanone	Valid		
TSCATS	3-Heptanone, 5-methyl-	Valid		

Other Sources

Other Sources	Synonym	Synonym Quality	Effective Date	End Date
CA Index	3-Heptanone, 5-methyl-	Valid		
CUS98	3-Heptanone, 5-methyl-	Valid		
ChemIDStd	5-Methyl-3-heptanone	Valid		
FDA	5-METHYL-3-HEPTANONE	Unknown		
NJ-RTK-HS	Ethyl sec-amyl ketone	Valid		

Ad Hoc List

There are no Synonyms of this type.

EPA Synonyms

There are no Synonyms of this type.

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Component Of

Systematic Name	Synonym	CAS Number	TSN	EPA Identifier	Effective Date	End Date
Volatile organic compounds	VOCs			E761346		

Related References

<http://www.osha.gov/dts/sltc/methods/organic/org007/org007.html>

http://www.osha.gov/dts/chemicalsampling/data/CH_239900.html

<http://nj.gov/health/eoh/rtkweb/documents/fs/0848.pdf>

<http://yosemite.epa.gov/oppts/epatscat8.nsf/ReportSearch?OpenAgent&CASNumber=541-85-5>

<http://chem.sis.nlm.nih.gov/chemidplus/direct.jsp?regno=541-85-5&result=advanced>

<http://chem.sis.nlm.nih.gov/chemidplus/direct.jsp?regno=0000541855>