

# Data contents in PubChem

## Laboratory Chemical Safety Summary (LCSS)

- As of October 30, 2015
- Abbreviations in brackets indicate data sources.

### GHS Classification [CLP, ICSC]

### Synonyms [PC]

### Identifiers

PubChem CID [PC]  
CAS [DRGBNK, EPA-CDR, ICSC, NIOSH, OSHA]  
InChi [PC]  
InChi Key [PC]

### Physical Properties

Physical Description [CAMEO, EPA-CDR, ICSC, NIOSH, OSHA]  
Odor [HSDB]  
Boiling Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]  
Melting Point [CAMEO, DRGBNK, HSDB, ICSC, NIOSH, OSHA]  
Flash Point [HSDB, ICSC, NIOSH, OSHA]  
Solubility [CAMEO, DRGBNK, HSDB, ICSC, NCI, NIOSH]  
Density [CAMEO, HSDB, ICSC, NIOSH, OSHA]  
Vapor Density [CAMEO, HSDB, ICSC, OSHA]  
Vapor Pressure [CAMEO, HSDB, ICSC, NIOSH, OSHA]  
Auto-Ignition [HSDB, ICSC]  
Decomposition [HSDB, ICSC]  
Corrosivity [HSDB]  
Odor Threshold [HSDB]

### Toxicity Data

Toxicity Summary [DRGBNK, HSDB]  
Human Toxicity Values [HSDB]  
Non-Human Toxicity Values [HSDB]

### Exposure Limits

Immediately Dangerous to Life or Health Concentration [NIOSH, OSHA]  
Recommended Exposure Limit (REL) [NIOSH, OSHA]  
Permissible Exposure Limit (PEL) [NIOSH, OSHA]  
REL-Time-Weighted Average Concentration (REL-TWAC) [OSHA]  
REL-Short-Term Exposure Limit (REL-STEL) [OSHA]  
REL-Ceiling (REL-C) [OSHA]  
PEL-Time-Weighted Average Concentration (PEL-TWAC) [OSHA]  
PEL-Short-Term Exposure Limit (PEL-STEL) [OSHA]  
PEL-Ceiling (PEL-C) [OSHA]  
Threshold Limit Values [HSDB]  
Occupational Exposure Limits [ICSC]  
Effects of Short Term Exposure [ICSC]  
Effects of Long Term Exposure [ICSC]  
Explosive Limits and Potential [HSDB, ICSC]  
Radiation Limits and Potential [HSDB]  
Acceptable Daily Intakes [HSDB]  
Allowable Tolerances [HSDB]

### Health and Symptoms

Symptoms [NIOSH]  
Carcinogen [ATSDR, HSDB, OSHA]  
Exposure Routes [ICSC, NIOSH]  
Target Organs [ATSDR, NIOSH]  
Cancer Sites [NIOSH]  
Fire Hazard [ICSC]  
Explosion Hazard [ICSC]  
Exposure Hazard [ICSC]  
Skin Hazard [ICSC]  
Inhalation Hazard [ICSC]  
Eye Hazard [ICSC]  
Ingestion Hazard [ICSC]  
Hazards Summary [ATSDR, EPA-AT, HSDB]  
Fire Potential [HSDB]  
Skin, Eye, and Respiratory Irritations [HSDB]

### First Aid

Fire First Aid [ICSC]  
Explosion First Aid [ICSC]  
Exposure First Aid [ICSC]  
Inhalation First Aid [ICSC]  
Skin First Aid [ICSC]  
Eye First Aid [ICSC]  
Ingestion First Aid [ICSC]

### Flammability and Explosivity

Flammability [HSDB, NIOSH]  
Lower Explosive Limit (LEL) [NIOSH, OSHA]  
Upper Explosive Limit (UEL) [NIOSH, OSHA]  
NFPA Hazard Classification [HSDB]  
NFPA Fire Rating [CAMEO, OSHA]  
NFPA Reactivity Rating [CAMEO, OSHA]  
NFPA Health Rating [CAMEO, OSHA]  
NFPA Other [CAMEO, OSHA]  
Critical Temperature [HSDB]  
Critical Pressure [HSDB]

### Stability and Reactivity

Reactivities and Incompatibilities [HSDB, NIOSH, OSHA]

### Storage and Handling

Safe Storage [ICSC]  
Storage Conditions [HSDB]  
Protective Equipment and Clothing [HSDB]  
Personal Protection [NIOSH]  
Respirator Recommendations [NIOSH]  
Nonfire Spill Response [OSHA]

### Cleanup and Disposal

Spillage Disposal [ICSC]  
Cleanup Methods [HSDB]  
Disposal Methods [HSDB]

### Additional Considerations

Toxic Combustion Products [HSDB]  
Other Hazardous Reactions [HSDB]

### ❖ Data Source Abbreviations

- ATSDR = CDC ATSDR Toxic Substance Portal
- CAMEO = NOAA CAMEO Chemicals
- CLP = Regulation (EC) No 12 1272/2008
- DRGBNK = DrugBank
- EPA-AT = EPA Air Toxics
- EPA-CDR = EPA Chemical Data Report
- HSDB = Hazardous Substances Data Bank
- ICSC = ILO International Chemical Safety Cards
- NCI-ID = NCI Investigational Drugs
- NIOSH = NIOSH Pocket Guide
- OSHA = OSHA Occupational Chemical DB
- PC = PubChem