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ROBUST SUMMARY FOR HFC-23

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Summary

HFC-23 is used as a refrigerant, as an etchant of silicon dioxide dielectric layers, and as a clean agent fire extinguishant. HFC-23 is a clear, colorless gas with a slight ethereal odor. It has a boiling point of -82°C and a melting point of -155.1°C (DuPont, 1992; Lide, 2001). HFC-23 has a density of 1.44 g/cm^3 at -82°C and a vapor density of 2.4 (air=1) (DuPont, 2002a; 2002b). HFC-23 has a vapor pressure of 45850 hPa at 25°C , an experimental log Kow of 0.64, and water solubility of 0.1 wt% at 25°C (DuPont, 1992; DuPont, 2002a; 2002b; Hansch et al., 1995; SRC, 2004). HFC-23 has no flash point. No further testing for physical-chemical properties is recommended.

HFC-32, difluoromethane, was selected as an analogous chemical for repeated dose and reproductive toxicity, based on its close physical-chemical properties and similar acute toxicity to HFC-23. The major properties of HFC-23 and HFC-32 are compared in Table 1.

Table 1: Comparison of Properties of HFC-23 and HFC-32

Chemical Name	Trifluoromethane	Difluoromethane
Synonym:	HFC-23	HFC-32
CAS#	75-46-7	75-10-5
Molecular Formula	CHF_3	CH_2F_2
Molecular Weight	70.01	52.02
Melting Point ($^{\circ}\text{C}$)	-155.1	-136
Boiling Point ($^{\circ}\text{C}$)	-82	-52
Vapor Pressure (25°C)	45850 hPa	16800 hPa
Heavier than Air?	Yes	Yes
4-hour ALC in rats study (ppm)	> 663,000	~760,000

If released to the atmosphere, HFC-23 is expected to exist solely as a vapor in the ambient atmosphere with an estimated half-life of about 180 years (Atkinson, 1989; SRC, n.d.). Some HFC-23 may gradually diffuse into the stratosphere with a diffusion half-life for transport from the troposphere to the stratosphere in the order of 20 years (Dilling, 1982). HFC-23 has a global warming potential (GWP) of 11,700 compared to the GWP of carbon dioxide and methane, which are 1 and 23, respectively. Hydrolysis is not expected to be an important process based on estimated half-lives of 5.1 years and

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190 days at pH values of 7 and 8, respectively (Mill et al., 1987; SRC, n.d.). HFC-23 is expected to have high mobility in soil and volatilization of HFC-23 from moist soil surfaces is expected to be an important fate process. The potential for volatilization of HFC-23 from dry soil surfaces may exist (SRC, n.d.). HFC-23 is not expected to adsorb to suspended solids and sediment in water and is expected to volatilize rapidly from water surfaces. The estimated volatilization half-life from a model river and lake are approximately 2.5 hours and 3.3 days, respectively (Lyman et al., 1990; SRC, n.d.). HFC-23 is not expected to biodegrade rapidly. No degradation was detected in a 24-hour bottle assay (King, 1997; Streger et al., 1999). A BCF of 3.2 was calculated for HFC-23, suggesting that bioconcentration in aquatic organisms is low (SRC, n.d.). No further environmental fate testing is recommended.

No ecotoxicological studies have been conducted with HFC-23 and there is very little or no ecotoxicology data for similar non-chlorinated, fluorocarbon compounds. The related compounds HFC-134a (1,1,1,2-tetrafluoroethane) and HFC-125 (1,1,1,2,2-pentafluoroethane) have been included here for comparison with HFC-23 as they are both fluorinated ethane substances, and test data for HFC-134a are available. ECOSAR was used to predict the aquatic toxicity of these fluorocarbons to green algae, daphnids (planktonic freshwater crustaceans), and fish (Table 2). ECOSAR predictions are based on actual toxicity test data for classes of compounds with similar modes of action, i.e., narcosis in the case of fluorocarbons. Predicted \log_{10} Kow values were used as input for the ECOSAR model. To help gauge the sensitivity of the prediction to this parameter, ECOSAR predictions were made using 2 Kow values. The initial Kow value was based on the estimated value from the Syracuse Research Corporation model except for the measured value of 0.64 for HFC-23 (Hansch et al., 1995). The second Kow value was empirically selected to be approximately \log_{10} 0.5 greater than the initial measured or estimated value.

Table 2: Aquatic Toxicity Values

Compound	\log_{10} Kow (Estimated)	Algae, 96-hr EC ₅₀ (Estimated)	Daphnid, 48-hr EC ₅₀ (Estimated)	Fish, 96-hr LC ₅₀ (Estimated)
		(mg/L)	(mg/L)	(mg/L)
HFC-23 (Trifluoromethane) (CHF₃)	0.64* 1.5	557 96	961 159	985 153
HFC-134a (1,1,1,2-Tetrafluoroethane) (C ₂ H ₂ F ₄)	1.5 2.0	140 51	231 81	223 76
HFC-125 (1,1,1,2,2-Pentafluoroethane) (C ₂ HF ₅)	1.5 2.0	165 60	272 95	263 89
* experimental value				

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The only test data available are for HFC-134a. Results of aquatic testing of HFC-134a with daphnids and fish indicated that the daphnid 48-hour EC_{50} was 980 mg/L and the 96-hour fish LC_{50} was 450 mg/L (Stewart and Thompson, 1991; Thompson, 1991). ECOSAR over predicts the toxicity of HFC-134a since the estimated EC/LC50 values (223, 231 mg/L) are a factor of 2-4 times lower than the empirical values. ECOSAR toxicity for HFC-23 is also likely to be over-estimated by ECOSAR. The measured log Kow of 0.64 for HFC-23 was used to estimate toxicity values for HFC-23. Based on the ECOSAR predictions, the actual toxicity test data for HFC-134a, and the high Henry's Law Constant for these compounds, HFC-23 is considered a low hazard to aquatic organisms. No further ecotoxicological testing is recommended.

The 4-hour inhalation ALC of HFC-23 in male rats was >663,000 ppm, and the 4-hour ALC of HFC-32 (analogous chemical) was ~ 760,000 ppm (DuPont, 1975; 1980). In cardiac sensitization studies in dogs, HFC-23 was found to have no potential to cause cardiac sensitization in beagle dogs at concentrations up to 30% in air or 50% in air with auxiliary oxygen. There were no positive responses, no questionable positive responses, and no ventricular tachycardia ectopic bursts (DuPont, 1993). No further acute toxicity testing is recommended.

Neuro-behavioral and physiological effects of HFC-23 were examined in 6 male volunteers. Individuals were exposed to 10, 20, 40, or 60% of HFC-23 at escalating concentrations administered as 8 pulses of 3 minutes each, with 2-minute clearance periods between each pulse. The first subject exposed to HFC-23 completed the 8 pulses, but experienced an anesthetic effect and nausea at 60%. Although other physiologic parameters remained stable, the subject's response was considered intolerable. The second subject to inhale 40% HFC-23 experienced discomfort after 1 minute, and requested discontinuation of exposure. Both the 40 and 60% levels were then dropped from further evaluation. The remaining 4 subjects tolerated the 30% level of HFC-23. Therefore, 30% was considered to be the MTC (maximum tolerated dose). At 30% subjects reported anesthetic effects, but no effects were noted in blood pressure, heart rate or rhythm, oxygenation, respiratory rate, temperature, end tidal CO_2 , or serum chemistries. However, when one subject received the 30% concentration during an NMR imaging study, an anesthetic effect with intolerable hyperacusis was demonstrated. In addition, exposure to 30% HFC-23 had systematic effects on neuropsychological functioning, mood, and subjective mental state (Fagan et al., 1995; Henry Ford, 1992; Rahill et al. 1998).

Although 90-day repeated dose inhalation studies with HFC-23 in rats and dogs reported LOAELs of > 10,000 and >5,000 ppm, respectively, there were insufficient details to assess the reliability of the studies (Leuschner et al., 1983). Therefore, data from an analogous chemical, HFC-32, are being presented to fulfill the repeated dose toxicity end point. A GLP 90-day inhalation toxicity study with HFC-32 was carried out in accordance with OECD Guideline No. 413. Groups of rats (20 per sex) were exposed whole body to HFC-32 for 6 hours per day, 5 days per week for 13 weeks. The treatment of rats with 4940, 14,600 and 49,100 ppm HFC-32 for 90 days resulted in a few minor and biologically insignificant changes (Ellis et al., 1996). Based on above data, no further repeated dose testing is recommended.

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In a developmental toxicity study, pregnant rats were exposed by inhalation to 0, 5000, 20,000 or 50,000 ppm HFC-23 for 6 hours per day, on days 7-21 of gestation. The maternal and developmental no-observed-effect level (NOEL) was 50,000 ppm, which was the highest dose tested. No further developmental toxicity testing is recommended (DuPont, 1997).

Although no histological effects were reported in reproductive organs in 90-day inhalation studies in rats and dogs, there were insufficient details to assess the reliability of these studies (Leuschner et al., 1983). Therefore, data from an analogous chemical, HFC-32, are being presented to fulfill the reproductive toxicity end point. In the 90-day inhalation toxicity study with HFC-32 no effects on any reproductive organs examined or testis weights were observed (Ellis et al., 1996). Based on the available data, it is unlikely that HFC-23 will affect fertility. Therefore, no further reproductive toxicity testing is recommended.

HFC-23 was neither mutagenic in *Salmonella typhimurium* (Ames assay) nor in a gene mutation assay in Chinese hamster ovary (CHO) AS52/XPRT cells (gpt locus) (US Army, 1996a; 1996b). HFC-23 was mutagenic in an *in vitro* chromosome aberration assay in CHO-K1 cells at concentrations of 80% to 100% in the absence of metabolic activation. Damage, however, was probably due to a decreased oxygen level rather than the activity of HFC-23, as under these same conditions 100% nitrogen also induced a significant increase in chromosomal damage to the same magnitude (US Army, 1996c). HFC-23 was positive in a *Drosophila* sex-linked recessive lethal (SLRL) test (Foltz and Fuerst, 1974). This study was included in the US EPA Report of the Gene-Tox Program, where HFC-23 could not be classified as positive or negative because of inadequate sample size. HFC-23 was negative in an *in vivo* mouse micronucleus assay (US Army, 1996d). No further genetic toxicity testing is recommended.

Human Exposure

HFC-23 is produced as a co-product in the reactors along with the production of HCFC-22 at the Louisville Works Plant site in Louisville, KY. The HFC-23 produced varies depending upon the age of the reactor catalyst, but is typically between 1% and 2% of the HCFC-22 produced. HCFC-22 is produced year round in the plant, so the HFC-23 is continuously produced along with the HCFC-22. The potential for exposure is greatest during loading of the material or during unscheduled maintenance. The primary concern for exposure is frostbite. The PPE for normal operations is Monogoggles and rubber gloves. If the exposure potential is likely due to line breaks containing residual material a Level "B" acid suit is worn (Greylite 20, a Poly Vinyl Chloride Material). For extreme potential exposure situations or emergency response a Greylite 20 Level "A" suit is worn.

In support of DuPont's commitment to reduce green house gas emission, the site has worked to minimize production of HFC-23 and improve HFC-23 capture technology. The Louisville plant has reduced emissions of HFC-23 about 70% from the 1990 base year. The HFC-23 is recovered into storage tanks and either sold into the fire extinguishant business or etchant gas business. More HFC-23 is produced than is sold, so the excess is shipped by railcar to Washington Works for destruction in their Thermal Converter. Losses of HFC-23 are minimized as much as possible by design. All of the

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HFC-23 processing equipment is located outdoors, so natural ventilation prevents accumulation of any high concentrations of HFC-23 where that material may leave the process (via small leaks or small vents necessary by design).

Because of its high vapor pressure, HFC-23 is handled as a liquefied gas during shipping and handling. Therefore, HFC-23 is handled in closed pressurized systems so that exposure typically does not occur except for during maintenance or an abnormal situation, such as a leak.

HFC-23 is marketed as Freon[®] 23 and is a blend component in SUVA[®] 95, which are both refrigerants for very low temperature applications such as medical freezers and environmental chambers, Zyron[®] 23, an etchant gas for the semiconductor industry, and as FE-13, a clean agent fire extinguishant.

The DuPont Acceptable Exposure Limit for HFC-23 is 1000 ppm (8- and 12-hour TWA).

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