4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

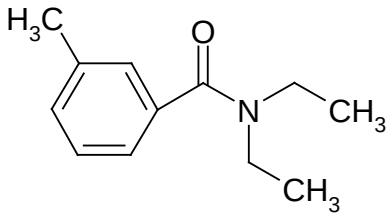
Information regarding the chemical identity of DEET is located in Table 4-1.

DEET is the chemical, N,N-diethyl-*meta*-toluamide, *ortho* and *para* isomers are present at low concentrations. DEET is an N,N-disubstituted aromatic carbonamide, which is used as an active ingredient in insect repellents. DEET was registered for commercial use by the general public in 1957. In December 1980, DEET was issued a Registration Standard (PB81-207722) followed by a Data Call-In in September 1988 requiring additional mammalian and avian toxicity data (EPA 1998c). Technical-grade DEET is typically formulated with carriers and solvents (such as ethanol, isopropanol, or water) for use in commercial products. Commercial product formulations include microencapsulated, pressurized sprays or aerosols, impregnated materials such as towelettes and roll-ons, and ready-to-use solutions such as non-aerosol pump sprays, liquids, creams, lotions, and foams. Some DEET products are also formulated with sunscreen. (EPA 2014l, 2014m; HSDB 2001). The DEET concentration in commercial products varies according to country and can range from 4 to 100% (by weight) in the United States. Technical-grade DEET typically contains 95% *meta*-isomer, the most effective form of the chemical (EPA 1998b, 1998c; O'Neil et al. 2013). The EPA does not require expiration dates to be included on the label of DEET products manufactured in the United States (EPA 1998b).

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of DEET is located in Table 4-2.

Table 4-1. Chemical Identity of DEET (N,N-Diethyl-*meta*-Toluamide)

Characteristic	Information	
Chemical name	N,N-Diethyl-*meta*-toluamide	
Synonym(s)	Benzamide, N,N-diethyl-3-methyl; N,N-diethyl-3-methylbenzamide; diethyltoluamide; diethyl toluamide; N,N-diethyl-*m*-toluamide; 3-methyl-N,N-diethylbenzamide; *m*-toluamide, N,N-diethyl; *m*-toluic acid diethylamide; *m*-delphene	ChemIDplus 2013; HSDB 2001
Registered trade name(s)	DEET; Delphene®; MGK diethyltoluamide; Detamide®; Detamine; Metadelphene®; Skeeter Skat®; Autan® (some formulations); Amincene C 140®; Amincene C-EM®; Bepper-DET®; DET®; DETA®; DET-20®; DETA-20®; Flypel®; Muscol®; Muskol®; Off!®; Repel®; Repper-DET®; Repudin-Special®; Chemform®; Cutter®; Old Time Woodsman®	ChemIDplus 2013; EPA 1998b, 1998c; HSDB 2001
Chemical formula	$C_{12}H_{17}NO$	HSDB 2001
Chemical structure		
Identification numbers:		
CAS registry	134-62-3	HSDB 2001
NIOSH RTECS	No data	
EPA hazardous waste	No data	
DOT/UN/NA/IMDG shipping	UN; IMO	
HSDB	1582	HSDB 2001
NCI	No data	
EPA Pesticide Chemical Code	080301	ChemIDplus 2013; HSDB 2001

CAS = Chemical Abstracts Service; DOT/UN/NA/IMDG = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of DEET

Property	Information	Reference
Molecular weight	191.27	HSDB 2001
Color	Nearly colorless liquid	EPA 1998b, 2012c
Physical state	Liquid	HSDB 2001
Melting point	-45°C -44.3°C	PhysProp 2014 Weeks et al. 2012
Boiling point	284-285°C 284.2°C 160°C at 19 mm Hg 111°C at 1.0 mm Hg 290°C 760 mm Hg	Weeks et al. 2012 ECHA 2010 HSDB 2001 O'Neil 2013 PhysProp 2014
Density:		
at 20°C/4°C	0.996 g/cm^3 1.01 g/cm^3 0.998 g/cm^3	HSDB 2001 Weeks et al. 2012 Weeks et al. 2012
Odor	Faint, characteristic odor	EPA 1998b, 2012c
Odor threshold:		
Water	No data	
Air	No data	
Taste threshold	No data	
Solubility:		
Water at 25°C	11,200 mg/L >1,000 mg/L at room temperature; 9,900 mg/L at 25°C	Weeks et al. 2012 CITI 1992; HSDB 2001 O'Neil et al. 2013
Organic solvent(s)	Miscible in benzene, carbon disulfide, chloroform, ethanol, ether, and isopropanol; soluble in hexane, acetonitrile, toluene, methylene chloride, and methanol; practically insoluble in glycerin	HSDB 2001; O'Neil et al. 2013; Weeks et al. 2012
Partition coefficients:		
Log K_{ow}	2.02 2.18 2.4 at 22°C and pH 6 2.66	Moody 1987; HSDB 2001 PhysProp 2014 ECHA 2010 CITI 1992; Weeks et al. 2012
K_{oc}	300 47–126	HSDB 2001 ECHA 2010; Weeks et al. 2012
Vapor pressure		
at 20°C	0.0056 mm Hg 0.00167 mm Hg at 25°C 0.00013 mm Hg at 25°C	HSDB 2001 O'Neil et al. 2013 Weeks et al. 2012
Henry's law constant	5.1 x10^{-8} atm-m^3/mol at 25°C	EPIWIN 2012
Autoignition temperature	No data	
Flashpoint	155°C 144°C	O'Neil et al. 2013 ECHA 2010

Table 4-2. Physical and Chemical Properties of DEET

Property	Information	Reference
Flammability limits	No data	
Explosive limits	No data	