

Appendix B

Chemical and Product Class Information for the Substances Tested in the ICE Test Method

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Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
Acetaldehyde	75-07-0	Aldehyde	Manufacture of acetic acid, perfumes, and flavors; Narcotic	liquid	S	100%	99%
Acetic acid	64-19-7	Carboxylic acid	Reagent; Indicator	liquid	S	10%	99%
Acetone	67-64-1	Ketone	Solvent; Antiseptic; Chemical intermediate; Raw material	liquid	S	100%	99%
Ammonium nitrate	6484-52-2	Inorganic salt, Onium compound	Fertilizer; Chemical intermediate; Industrial explosive	solid	S	100%	>99.9%
L-Aspartic acid	70-47-3	Amino acid	Organic intermediate; Fungicides; Germicides	solid	S	100%	100%
Benzalkonium chloride (1%)	8001-54-5	Onium compound	Surfactant (cationic), Bactericide, Fungicide, Preservative	liquid	S	1, 5, 10 and 100%	98%
Brij 35	9002-92-0	Alcohol	Solvent; Excipient; Surfactant	n.p.	S	100%	n.p.
Butanol	71-36-3	Alcohol	Ingredient of spray paint; Nail polish	liquid	S	100%	99%
n-Butyl acetate	123-86-4	Ester	Solvent; Synthetic flavor ingredient	liquid	I *	100%	99%
2-Butoxyethyl acetate	112-07-2	Alcohol	Cleaner; Polish; Sealant	liquid	n.p.	100%	99%
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	S	100%	90%
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Manufacturing impurity (polyester); Developer intermediate	solid	I*	100%	95%
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Onium compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	Sf	0.1, 6 and 10%	98%
Chlorhexidine	55-56-1	Amine/Amidine	Disinfectant; Mouthwash; Anti-infective agent	solid	I*	100%	n.p.
Chloroform	67-66-3	Hydrocarbon (halogenated)	Solvent; Cleaner	liquid	I*	100%	99.8%
Cyclohexanol	108-93-0	Alcohol	Solvent; Chemical intermediate	liquid	S	100%	97%
Cyclohexylamino-functional PMS	↓	Organosilicon compound	↓	liquid	n.p.	↓	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
Decamethylcyclopentasiloxane	541-02-6	Organosilicon compound	Ingredient of hair conditioner; Diaper rash ointment; Car wax	liquid	n.p.	↓	n.p.
Dibenzoyl-L-tartaric acid	2743-38-6	Carboxylic acid, Ester	Optical resolution agent	solid	I	100%	98%
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	I*	100%	99%
Dibutyltin dichloride	683-18-1	Organometallic compound	Industrial chemical; Immunosuppressive agent	solid	S	100%	97%
2,6-Dichlorobenzoyl chloride	4659-45-4	Acyl halide	Anti-infective; Anti-fungal; Preservative	liquid	I*	100%	99%
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	I	100%	96%
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals; Pesticides; perfumes	solid	I	100%	99.5%
Dimethyl sulfoxide	67-68-5	Organic sulfur compound	Solvent; Cryoprotective agent	liquid	S	100%	99.9%
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	S	100%	n.p.
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	S	100%	99%
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	S	100%	99%
Ethyl-2-methylacetoacetate	609-14-3	Ketone, Ester	Not classified	liquid	S*	100%	97%
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	I*	100%	99%
Fomesafen	72128-02-0	Imide, Ether, Nitro compound	Pesticide	solid	S	100%	97.5%
Gammabutyrolactone	96-48-0	Heterocyclic, Lactone	Synthetic intermediate; Solvent	liquid	S	100%	>99%
Glycerol	56-81-5	Alcohol	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle	liquid	S	100%	>99%
n-Hexane	110-54-3	Hydrocarbon (acyclic)	Solvent; Adhesive; Gasoline additive	liquid	I	100%	99%
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	I*	100%	98%
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	S	100%	99%

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	I*	100%	99.9%
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)	liquid	S	100%	99.9%
Maneb	12427-38-2	Amine/Amidine, Organic salt, Urea compound	Pesticide	solid	S	100%	90%
Mercury (II) chloride	7487-94-7	Inorganic chloride compound	Antiseptic; Disinfectant	solid	I	100%	99.5%
2-Methoxyethanol	109-86-4	Alcohol	Solvent	liquid	S	100%	99.9%
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	S	100%	98%
Methyl cyanoacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	S*	100%	99%
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	S	100%	99%
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Drycleaning	liquid	I*	100%	98%
Methylcyclopentane	96-37-7	Hydrocarbon (cyclic)	Solvent	liquid	I*	100%	>99%
1-Naphthaleneacetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	I*	100%	96%
1-Naphthaleneacetic acid, sodium salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	S*	100%	95%
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	I*	100%	>99%
Parafluoroaniline	371-40-4	Amine/Amidine	Intermediate for herbicides; Dyes	liquid	I	100%	99%
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	S	100%	n.p.
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	S	100%	97%
Promethazine HCl	58-33-3	Amine/Amidine, Heterocyclic, Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	S*	100%	98%

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	S	100%	>99.9%
Quinacrine	69-05-6	Amine/Amidine, Heterocyclic, Polycyclic compound	Anti-infective (anti-helmentic)	solid	S*	100%	n.p.
Silver (I) nitrate	7761-88-8	Inorganic silver/nitrogen compound	Anti-infective; Diagnostic agent	solid	S	3%	99%
Sodium dodecyl sulfate	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	solid	Sf	100%	70%
Sodium fluorescein	518-47-8	Polycyclic	Stain; Dye	liquid	S	20%	70.0%
Sodium hydroxide	1310-73-2	Alkali	Caustic agent	liquid	S	1%	n.p.
Sodium hydroxide	1310-73-2	Alkali	Caustic agent	liquid	S	1 and 10%	RG
Sodium lauryl sulfate	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	Sf	3 and 15%	98%
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic, Industrial byproduct	solid	S	100%	>99%
Sodiumperborate, 4H ₂ O	10486-00-7	Inorganic salt, Boron compound	Household cleaner; Detergent	solid	S	100%	98.6%
Tetraaminopyrimidine sulfate	5392-28-9	Amine/Amidine, Heterocyclic	Developer	solid	I*	100%	97%
TNO-01 (Formulation-1)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-02 (Formulation-2)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-03 (Pesticide-1)	n.p.	Not classified	Pesticide	liquid	n.p.	undiluted	n.p.
TNO-04 (Detergent-1 ¹²)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-05 (Silicone powder-1)	n.p.	Not classified	Not classified	solid	I	undiluted	n.p.
TNO-06 (Lubricant)	n.p.	Not classified	Not classified	gel	n.p.	undiluted	n.p.
TNO-07 (Ink-1)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-08 (Ink-2)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-09 (Paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
TNO-10 (Silicone powder-2)	n.p.	Not classified	Not classified	solid	I	undiluted	n.p.
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	Hydrocarbon; Acid	Industrial chemical	solid	n.p.	undiluted	n.p.
TNO-12 (Formulation-3)	n.p.	Not classified	Not classified	paste	n.p.	undiluted	n.p.
TNO-13 (Pesticide-2)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-14 (Polydisaccharide)	n.p.	Carbohydrate	Not classified	liquid	n.p.	14.5%	n.p.
TNO-15 (Polydisaccharide)	n.p.	Carbohydrate	Not classified	liquid	n.p.	50%	n.p.
TNO-16 (Liquid nylon product)	n.p.	Not classified	Industrial formulation	liquid	n.p.	undiluted	n.p.
TNO-17 (Solvent-1)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
TNO-18 (Solvent-2)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-19 (Solvent-3)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-20 (Solvent-4)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-21 (Solvent-5)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-22 (Solvent-6)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-23 (Solvent-7)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-24 (Solvent-8)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-25 (Solvent-9)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-26 (Ink-3)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-27 (Thermal paper coating-1)	n.p.	Not classified	Industrial chemical	liquid	n.p.	undiluted	n.p.
TNO-28 (Toilet cleaner-1)	n.p.	Not classified	Household cleaner	liquid	n.p.	undiluted	n.p.
TNO-29 (Toilet cleaner-2)	n.p.	Not classified	Household cleaner	liquid	n.p.	undiluted	n.p.
TNO-30 (Pesticide-3)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-31 (Sulfur)	7704-34-9	Inorganic chemical	Industrial chemical	solid	I	undiluted	n.p.
TNO-32 (Ink-4)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-33 (Thermal paper coating-2)	n.p.	Not classified	Industrial chemical	liquid	n.p.	undiluted	n.p.
TNO-34 (Detergent-2)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-35 (Propyl-lactate)	616-09-1	Acid	Food additive; Solvent	liquid	S	undiluted	n.p.
TNO-36 (Ethylhexyl lactate)	6283-86-9	Acid; Ester	Solvent; Wetting agent	liquid	n.p.	undiluted	n.p.
TNO-37 (Pesticide-4)	n.p.	Not classified	Pesticide	solid	n.p.	undiluted	n.p.
TNO-38 (Solvent-10)	n.p.	Not classified	Solvent	liquid	n.p.	undiluted	n.p.
TNO-39 (Detergent-3)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-40 (Glycolbromoacetate form)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-41 (Amidosulfonic acid)	5329-14-6	Acid	Herbicide; Flame retardant; Metal cleaning; Acid dye	solid	n.p.	100%	n.p.
TNO-42 (Glycolbromoacetate)	3785-34-0	Acetate	Not classified	liquid	n.p.	85%	n.p.
TNO-43 (Monobromoacetic acid)	79-08-3	Acid	Chlorination byproduct	solid	S	undiluted	n.p.
TNO-44 (Didecyldimethylammonium chloride [23% in propyl glycol])	7173-51-5	Not classified	Household cleaner (disinfectant)	liquid	n.p.	23%	n.p.
TNO-45 (Aqueous framing solution)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-46 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-47 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-48 (Corrosion inhibitor liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-49 (Wood impregnator liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-50 (Sodium hypochlorite-containing formulation)	n.p.	Not classified	Disinfectant	n.p.	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
TNO-51 (Disinfectant)	n.p.	Not classified	Disinfectant	n.p.	n.p.	undiluted	n.p.
TNO-52 (Pesticide liquid)	n.p.	Not classified	Pesticide	liquid	n.p.	undiluted	n.p.
TNO-53 (Ink formulation)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-54 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-55 (Elastomer liquid)	n.p.	Not classified	Elastomer	liquid	n.p.	undiluted	n.p.
TNO-56 (Elastomer liquid)	n.p.	Not classified	Elastomer	liquid	n.p.	undiluted	n.p.
TNO-57 (Epoxy resin liquid)	n.p.	Not classified	Resin	liquid	n.p.	undiluted	n.p.
TNO-58 (Styrene resin powder)	n.p.	Not classified	Resin	solid	n.p.	undiluted	n.p.
TNO-59 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-60 (Fungicide paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
TNO-61 (Silver thiosulfate liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-62 (Lactate liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-63 (Copolymer powder)	n.p.	Not classified	Copolymer	solid	n.p.	undiluted	n.p.
TNO-64 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-65 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-66 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-67 (Ink formulation)	n.p.	Not classified	Dyes	liquid	n.p.	undiluted	n.p.
TNO-68 (Cleaning product)	n.p.	Not classified	Cleaner	liquid	n.p.	undiluted	n.p.
TNO-69 (Cleaning product)	n.p.	Not classified	Not classified	liquid	n.p.	2%	n.p.
TNO-70 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-71 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-72 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-73 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	emulsion	n.p.	undiluted	n.p.
TNO-74 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-75 (Fluoroallyl acrylate copolymer)	n.p.	Not classified	Copolymer	liquid	n.p.	undiluted	n.p.
TNO-76 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-77 (Raw material liquid)	n.p.	Not classified	Raw material	liquid	n.p.	undiluted	n.p.
TNO-78 (Raw material liquid)	n.p.	Not classified	Raw material	liquid	n.p.	undiluted	n.p.
TNO-79 (Silicon resin powder)	n.p.	Not classified	Silicone resin	solid	n.p.	undiluted	n.p.
TNO-80 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.

Substance	CASRN	Chemical Class	Product Class	Form Tested	Water Solubility ₁	Concentration Tested	Purity ²
TNO-81 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-82 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-83 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-84 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-85 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-86 (Surfactant liquid)	n.p.	Not classified	Soaps; Surfactants	liquid	n.p.	undiluted	n.p.
TNO-87 (Enzyme liquid)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-88 (Miscellaneous liquid)	n.p.	Not classified	Not classified	liquid	n.p.	undiluted	n.p.
TNO-89 (Ferro powder)	n.p.	Not classified	Not classified	solid	n.p.	undiluted	n.p.
TNO-90 (Enzyme solution)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-91 (Enzyme solution)	n.p.	Not classified	Enzyme solution	liquid	n.p.	undiluted	n.p.
TNO-92 (Raw material powder)	n.p.	Not classified	Raw material	solid	n.p.	undiluted	n.p.
TNO-93 (Antifouling paint)	n.p.	Not classified	Paint	emulsion	n.p.	undiluted	n.p.
TNO-94 (Antifouling paint)	n.p.	Not classified	Paint	liquid	n.p.	undiluted	n.p.
Toluene	108-88-3	Hydrocarbon (cyclic)	Solvent; Gasoline additive; Manufacture of benzene derivatives, medicines, dyes, perfumes	liquid	I *	100%	99%
Triacetin	102-76-1	Lipid	Anti-fungal	liquid	I*	100%	99%
Tributyltin chloride	1461-22-9	Organometallic compound, Heavy metal	Pesticide; Preservative	liquid	n.p.	100%	96%
Trichloroacetic acid	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	S	3 and 30%	RG
Triethanolamine	102-71-6	Amine/Amidine, Alcohol	Cleaner; Cosmetic ingredient; Intermediate for herbicides, waxes, cutting oils	liquid	S	100%	99.9%
Triton X-100	9002-93-1	Polyether	Surfactant (nonionic), Detergent, Emulsifier	liquid	Sf	5 and 10%	98%
Triton X-500	↓	Polyether	Surfactant (nonionic), Detergent, Emulsifier	liquid	n.p.	5%	n.p.
Tween 20	9005-64-5	Ester, Polyether	Surfactant (nonionic), Detergent	liquid	Sf	100%	98%

¹I=Insoluble, S=Soluble, Sf=Surfactant, *=Solubility uncertain, n.p.=Not provided and not obtained

² n.p.=Not provided and not obtained, RG=Reagent grade