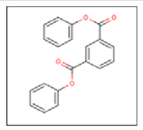
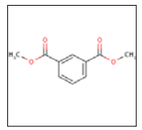
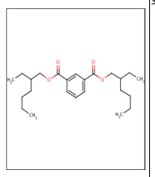
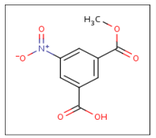
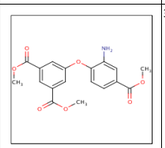
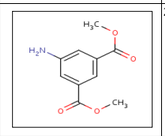
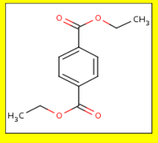
CERCLA Phthalate Ester Category
MA TURA Science Advisory Board Review
Appendix H2

Meta Para Phthalate Esters EHS Summary for June 26, 2014 SAB Meeting

Common Abbrev.	Common Chemical Name	CAS No.	TURA Listed	Chemical Name (Synonyms)	Chemical Formula	Structure Note: Boxes with yellow backgrounds indicate the para phthalate esters	Molecular Weight (mainly from ChemID Plus)	Viscosity in Centistokes (or otherwise noted) @ 20 deg C (HSDB, etc…)	Physical State at Room Temperature (HSDB, RTECS, CICAD, CHRIS)	Vapor Pressure mmHg at ~20C (HSDB, MSDS, ICSC)	PBT (from www.pbtprofiler.net)						IARC/CARC.	Neurotoxicity (Score card)	Other recognized (R) or suspected health effects (Scorecard/ MSDS)	Reproductive/Developmental Toxicity (On Prop 65 List?)	Target Organ (HAZMAP)			LD50 (ChemID Plus, RTECS)	LC50 (ChemID Plus, RTECS)	Flash Point (HSDB, MSDS, ICSC, CHRIS)	Reactivity (ICSC, MSDS, HSDB)	TYPES OF DATA AVAILABLE in RRD	Other R-phrases & H-Statements (REACH Registration Database)	H-Statements (CLP Database) Harmonized	Metabolites [CDC, HSDB]
											Water	Soil	Sediment	Air	BCF	Fish ChV					CNS	Liver	Other							
	Diphenyl isophthalate	744-45-6	No	1,3-Benzenedicarboxylic acid, 1,3-diphenyl ester	C20-H14-O4		318.327	n/a	solid [MSDS]	n/a	15	30	140	2.8	230	0.15	n/f	n/f	n/f	N	n/f	n/f	may cause eye/skin/resp irritation [MSDS]	n/f	n/f	433.4F [MSDS]	Incompatible with strong oxidizing agents; Haz Decomp Products = Carbon monoxide and carbon dioxide [MSDS]	N/F	N/F	Not harmonized = H315 (Skin Irrit. 2) and H319 (Eye Irrit. 2)	Some activity was noted by renal enzymes in the formation of monoester from the correspondlng diesters; only very weak activity for the cleavage of the monoesters was seen. Compared with the formation rate of terephthalic-acid from di-n-butyl-terephthalate, the rate of isophthalic-acid formation from di-n-butyl-isophthalate was more than twice as high with renal enzymes. Half ester formation rate was relatively rapid in all preparations. Acid formation was slow. This suggested that acid formation was the rate limiting step. [HSDB]
DMIP	Dimethyl isophthalate	1459-93-4	No	Dimethyl 1,3-benzenedicarboxylate	C10-H10-O4		194.185	n/a	Solid	0.00963 @ 25 deg C (est) [HSDB]	15	30	140	25	5.8	4	n/f	N	None Listed	N	N	Y	Eye Irr [HAZMAP]; may cause skin/resp irr [MSDS]	Oral, rat, 4390 mg/kg [HSDB]	n/f	280F c.c. [HSDB]	when heated to decomp it emits acrid smoke and fumes [HSDB]; Incompatible with strong oxidizing agents, avoid dust generation and excess heat, haz decomp products CO and CO2 [MSDS]	Read across on Repro/Develop.; Acute Tox, Irr, Sens, Rep Dose, Gen Tox, Repro, Dev, Carc	H319 - Eye Irrit. 2 Xi; R36 - Irritating to Eyes	Not harmonized = H315 (Skin Irrit. 2) and H319 (Eye Irrit. 2)	N/F
DOIP	Di-2-ethylhexyl isophthalate	137-89-3	No	Isophthalic acid, bis(2-ethylhexyl) ester	C24-H38-O4		390.56	86 centipoise [MSDS]	Liquid [NTP]	n/f	15	30	140	0.71	700	NE	n/f	n/f	n/f	N	n/f	n/f	skin/eye irritant [RTECS]	oral, rat, 17,300 uL/kg; dermal, rabbit 7,940 ul/kg [RTECS]	n/a	>200F [NTP]	Incompatible with oxidizing agents; Hazardous decomposition products "as with other organic materials, combustion will produce CO, CO2"; When heated to decomposition this chemical emits acrid smoke and irritating fumes. [NTP]	N/F	N/F	Not classified	Some activity was noted by renal enzymes in the formation of monoester from the correspondlng diesters; only very weak activity for the cleavage of the monoesters was seen. Compared with the formation rate of terephthalic-acid from di-n-butyl-terephthalate, the rate of isophthalic-acid formation from di-n-butyl-isophthalate was more than twice as high with renal enzymes. Half ester formation rate was relatively rapid in all preparations. Acid formation was slow. This suggested that acid formation was the rate limiting step. [HSDB - as CAS # 121-91-5]
	Methyl 5-nitrohydrogen.isophthalate	1955-46-0	No	1,3-Benzenedicarboxylic acid, 5-nitro-, 1-methyl ester	C9-H7-N-O6		225.16	Not relevant	Solid [MSDS]	n/a	15	30	140	21	3.2	46	n/f	n/f	n/f	N	n/f	n/f	n/f	Read Across data indicates oral, rat, 1387 mg/kg bw [RR]	Data waived [RR]	n/a	Avoid strong oxidizing agents, Hazardous decomposition products formed under fire conditions - Carbon oxides, Nitrogen oxides (N0x) [MSDS]	Acute Tox, Sens, Gen Tox, Repro	None found	Not harmonized = H315 (Skin Irrit. 2) ; H319 (Eye Irrit. 2); H335 STOT SE 3 (lungs - inhalation)	No record found
	n-pentyl-isopentylphthalate	84777-06-0	No	1,2-Benzenedicarboxylic acid, dipentyl ester, branched and linear; Diisopentylphthalate	$C_{18}H_{24}O_{4}$-2	No Structure in Chem Id Plus	306.4	n/f	n/f	n/f	Data not found							n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	When heated to decomposition it emits acrid smoke and irritating vapors.When heated to decomposition it emits toxic vapors of NOx and Cl–. [ONLINE]	None	Candidate List for SVHC - Toxic for Reproduction	Repr. 1B - H360FD; Aquatic Acute 1 H400 Repr. Cat. 2; R60-61 N; R50	No record found
	Dimethyl 5-[2-amino-4-(methoxycarbonyl)phenoxy] isophthalate	100596-38-1	No	1,3-Benzenedicarboxylic acid, 5-(2-amino-4-(methoxycarbonyl)phenoxy)-, dimethyl ester	C18-H17-N-O7		359.33	Not relevant	Solid [ONLINE]	n/f	Data not found							n/f	n/f	n/f	N	n/f	n/f	n/f	Oral, rat , >10000 mg/kg [RTECS]	n/f	211 deg C [ONLINE]	n/f	None	N/F	Not harmonized = H315 (Skin Irrit. 2) ; H319 (Eye Irrit. 2); H335 STOT SE 3	No record found
	Dimethyl 5-aminoisophthalate	99-27-4	No	5-Aminoisophthalic acid dimethyl ester	C10-H11-N-O4		209.2	n/f	Solid [MSDS]	n/f	15	30	140	2.8	2.6	0.65	n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	Avoid strong oxidizing agents, strong acids & bases; Hazardous decomposition products formed under fire conditions - Carbon oxides, nitrogen oxides (N0x) [MSDS]	None	N/F	Not harmonized = H315 (Skin Irrit. 2) ; H319 (Eye Irrit. 2); H335 STOT SE 3	No record found
	Diethyl terephthalate	636-09-9	No	Terephthalic acid, diethyl ester	C12-H14-O4		222.239	n/a	Solid [MSDS]	n/f	15	30	140	4.6	26	0.99	n/f	n/f	n/f	N	n/f	n/f	irr to eye/resp/skin [online]	n/f	n/f	243F [online]	Incompatible with oxidizing agents, haz decomp products = CO and CO2 [MSDS]	None	N/F	Not harmonized = H315 (Skin Irrit. 2) ; H319 (Eye Irrit. 2); H335 STOT SE 3 (na)(Inhalation)	No record found

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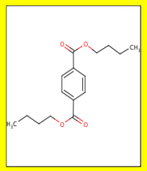
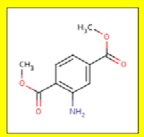
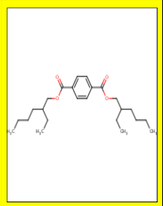
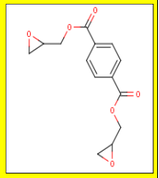
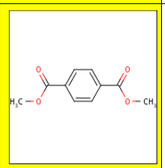
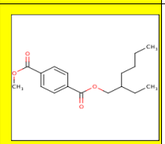
	Dibutyl terephthalate	1962-75-0	No	1,4-Benzenedicarboxylic acid, dibutyl ester	C16-H22-O4		278.35	16 mPa s (dynamic) @ 25 deg C [RR]	Liquid [RR]	< 0.038 Pa @ 25 deg C [RR]	8.7	17	78	1.8	2,100	0.048	n/f	n/f	n/f	N	n/f	n/f	n/f	Oral, rat, > 2,000 mg/kg bw [RR]; Intraperitoneal, mse, LDLo: 1392, mg/kg [RTECS]	n/f	196 deg C @ 101.325 kPa [RR]	Avoid strong oxidizing agents, Haz Decomp products CO2 and CO, Can decompose at elevated temperatures [MSDS]	Acute Tox, Sens, Gen Tox, Repro, Human	None found	Not classified	A Rhodococcus species was isolated from soil by enriching for growth with dimethyl terephthalate as the sole carbon source. The organism degraded dimethyl terephthalate by hydrolysis of ester-bonds to free terephthalic acid which in turn was metabolized through protocatechuate by an ortho-cleavage pathway. [HSDB] No evidence of metabolism of (14)C TPA was obtained by analysis of urine by high-performance liquid chromatography /following an iv dose to Fischer-344 rats/. [HSDB]
	Dimethyl 2-aminoterephthalate	5372-81-6	No	1,4-Benzenedicarboxylic acid, 2-amino-, dimethyl ester	C10-H11-N-O4		209.2	Not relevant	Solid [MSDS]	0.007 Pa (Est) [RR]	15	30	140	2	15	1.8	n/f	n/f	n/f	N	n/f	n/f	n/f	Oral, rat, >2000 mg/kg [RR]	n/f	n/a	Avoid strong oxidizing agents, Hazardous decomposition products formed under fire conditions - Carbon oxides, Nitrogen oxides (N0x) [MSDS]	Acute Tox, Sens, Gen Tox	H411 Aq Chronic 2; N; R51/53	Not harmonized = H315 (Skin Irrit. 2) ; H319 (Eye Irrit. 2); H335 STOT SE 3; Aq Chronic 2 H411	No record found
DEHT	Bis(2-ethylhexyl) terephthalate Dioctyl terephthalate Eastman 168-CA plasticizer avail studies [GreenScreen; Sids 2003]	6422-86-2	No	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	C24-H38-O4		390.56	63 cp at 25 deg C [HSDB]	Liquid [HAZMAP]	2.14X10-5 mm Hg at 25 deg C (est) [HSDB]	15	30	140	0.75	700	NE	n/f	N	N	N	N	N	May cause irritation [HAZMAP]	Oral, rat, >5,000 mg/kg; Dermal, guinea pig, >20ml/kg [Online MSDS]	LCLo (Rat, Inh, 6hr): >0.0718 mg/l [MSDS]	238 deg C or 460 deg F (open cup) [HSDB]	Avoid strong oxidizing agents, Haz	Carcinogenicity study, Acute Tox, Sens, Gen Tox, Repro	None found	Not harmonized; H413, H361	About 63% of the administered dose was metabolized to 2-ethylhexanol, mono-(2-ethylhexyl) terephthalate, and terephthalic acid and these compounds were absorbed from the gastrointestinal tract while the remainder of the dose was excreted unchanged in the feces. Di (2-ethylhexyl) terephthalate was metabolized predominantly to terephthalic acid. [ECHA database from 1984 industry study]
	Bis(2,3-epoxypropyl) terephthalate	7195-44-0	No	Terephthalic acid diglycidyl ester	C14-H14-O6		278.26	Data waived [RR]	Solid [RR]	<= 0.000068 Pa [RR]	15	30	140	3.3	3.2	0.54	n/f	n/f	n/f	N	n/f	n/f	n/f	Oral, rat, >2500 mg/kg [RR]; Oral, rat, >5000 mg/kg [RR]	Data waived [RR]	Data waived [RR]	Not flammable [RR]	Acute Tox, Sens, Gen Tox, Repro	H315: Skin Irrit. 2 H318: Eye Damage 1 H317: Skin Sens. 1 Xi; R41 (serious eye) R38 (skin irr) R43 Skin sens.	Not harmonized = H315 (Skin Irrit. 2) ; H317 Skin Sens. 1; H318 Eye Dam. 1; H319 (Eye Irrit. 2); H335 STOT SE 3 (lungs); Aq Chronic 2 H411	No record found
DMT	Dimethyl terephthalate	120-61-6	No	1,4-Benzenedicarboxylic acid, dimethyl ester	C10-H10-O4		194.2	Not relevant	Solid [HAZMAP]	0.01 mm Hg [HAZMAP]	15	30	140	28	14	3.3	n/f	N	N	N	N	N	Eye irritant; Causes urinary tract calculi in high dose animal studies; There are no published reports of human studies; [AIHA] -- [HAZMAP]	Oral, rat, 3200 mg/kg [RTECS]	Inh, rat, >6000 mg/m3/2H [RTECS]	141 deg C; [ICSC]--[HAZMAP]	The finely powdered ester is a significant dust explosion hazard; Incompatible with strong acids, bases, nitrates, and strong oxidizers. [HSDB]	None	None found	Not harmonized = H317 Skin Sens. 1; H319 (Eye Irrit. 2); H335 STOT SE 3 (organs); Aq Chronic 3 H412	Rat (terephthalic acid); Mouse (monomethyl terephthalate (70%), terephthalic acid (30%), and traces of DMT; ... Most of the absorbed DMT is metabolized to terephthalic acid (TPA) via hydrolysis, which sometimes combines with calcium to form TPA-Ca+2 precipitates. [HSDB]
	2-ethylhexyl methyl terephthalate	63468-13-3	No	n/f	C17-H24-O4		292.37	n/f	n/f	n/f	Data not found							n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	n/f	None	N/F	Nothing found in result	No record found
											Questions																			
	Tetraammonium 5-(4-(7-amino-1-hydroxy-3-sulfonato-2-naphthylazo)-6-sulfonato-1-naphthylazo)isophthalate	CAS# in EXPUB = NaN-30-5; EC #: 405-130-5	No	n/f	n/f	No record found in ChemID Plus	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	Acute Tox (oral/dermal); Rep dose tox; Gen Tox	H317 Skin Sens. 1 Xi; R43	H317 Skin Sens. 1 R43	No record found
	n-octadecylaminodiethyl hydrogen maleate hydrogenphthalate reaction mass of n-octadecylaminodiethyl bis(hydrogen maleate)	EC#: 405-960-8	No	n/f	n/f	No record found in ChemID Plus	n/f	n/f	Solid [RR]	<0.00005 Pa @ 25C [RR]	Data not found						n/f	n/f	n/f	N	n/f	n/f	n/f	>5,000 mg/kg bw [RR]	n/f	n/f	n/f	Acute Tox (oral/dermal); Rep dose tox	N; Xi; R43; R51/53	H317 Skin Sens. 1 H411 Aq. Chronic 2 R43 N; R51-53	No record found

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	A mixture of: sodium 5-[8-[4-[4-[4-[7-(3,5-dicarboxylatophenylazo)-8-hydroxy-3,6-disulfonatonaphthalen-1-ylamino]-6-hydroxy-1,3,5-triazin-2-yl]-2,5-dimethylpiperazin-1-yl]-6-hydroxy-1,3,5-triazin-2-ylamino]-1-hydroxy-3,6-disulfonatonaphthalen-2-ylazo]-isophthalate	CAS#: 187285-15-0 EC #: 413-180-4	No	n/f	n/f	No record in Chem ID Plus	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	n/f	Acute Tox (oral/dermal); Rep dose tox; Gen Tox [NONS designation - can't see data fully]	N/F	H318 Eye Dam. 1 Xi; R41	No record found
	O'-methyl O-(1-methyl-2-methacryloyloxy-ethyl)-1,2,3,6-tetrahydrophthalate	127244-43-3	No	n/f	n/f	No record in Chem ID Plus	n/f				**Data not found**						n/f	n/f	n/f	N	n/f	n/f	n/f					None	No results found	No results found	No record found
	Dimethyl 5-((4-Chlorobenzoyl)Amino) Isophthalate	349091-40-3	No	n/f	C17H14ClNO5	No record in Chem ID Plus	347.8	n/f	n/f	n/f	**Data not found**						n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	n/f	None	N/F	Not harmonized: Aq. Acute 1 H400	No record found
	Dimethyl 5-((1,2,3,4-Tetrahydro-9-AcridinylCarbonyl)Amino)Isophthalate	853317-87-0	No	n/f	n/f	No record in Chem ID Plus	n/f	n/f	n/f	n/f	**Data not found**						n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	n/f	None	N/F	Not harmonized: Eye Irrit. 2 H319; Aq Chronic 4 H413	No record found
	Dimethyl-5-tert-butylisophthalate	16308-65-9	No	n/f	C14H18O4	No record in Chem ID Plus	250.29	n/f	n/f	n/f	**Data not found**						n/f	n/f	n/f	N	n/f	n/f	n/f	n/f	n/f	n/f	n/f	None	N/F	Not harmonized: Acute Tox. 4 H302; Resp. Sens. 1 H334	No record found

Key: N = not on list or in database for this endpoint; n/a = not available; NE = Not estimated; n/f = not found; CAS = Chemical Abstract Service; CDC = U.S. Centers for Disease Control; CHRIS = Chemical Hazard Response Information System; CICAD = Concise International Chemical Assessment Documents from WHO = World Health Organization; CIDP = Chem ID Plus database; CLP = ECHA Classification, Labelling and Packaging database; HAZMAP = U.S. National Library of Medicine, Information on Hazardous Chemicals and Occupational Diseases; HSDB = Hazardous Substances Data Bank; ICSC = International Chemical Safety Card; IARC = International Agency for Research on Cancer; MSDS = Material Safety Data Sheet; NTP = National Toxicology Program; Online = Found on vendor website or other online resource; PBT = Persistent, Bioaccumulative, & Toxic; Prop 65 = CA Proposition 65 List of Carcinogenic, Reproductive and Developmental Toxicants; RRD or RR = REACH Registration Database; RTECS = Registry of Toxic Effects of Chemical Substances; TURA = Toxics Use Reduction Act.