

Electronic Supplementary Information for "Selection of a recyclable in situ liquid-liquid extraction solvent for foam-free synthesis of rhamnolipids in a two-phase fermentation", Demling et al. 2020
n.a. - not available or only for analytical application available

Solvent properties (20°C, 1.13 bar)												Price (list price)		Health Score			
Solvent name (IUPAC)	CAS	Suitable Solvent?	Density	source	Solubility	source	Boiling point	source	log K _{OW} -value	source	Flashpoint	source	Price (€/100ml)	source	date [DD.MM.YYYY]	Health Score	source
			[g/L]		[g/L]		[°C]				[°C]		€				
			880		0.3		100		4				100				
			920		0.5		80		3.5				120				5
ethyl decanoate	110-38-3	unrestricted	862	www.chemspider.com	1.59E-02	www.pubchem.com	241.5	www.pubchem.com	4.79	www.chemspider.com	104	Merck KGaA, Darmstadt,	23.00	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
ethyl (Z)-octadec-9-enoate	111-62-6	unrestricted	870	www.chemspider.com	5.79E-07	www.chemspider.com	217	www.chemspider.com	8.51	www.chemspider.com	>103	Deutsche Gesetzliche Un	47.67	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
methyl decanoate	110-42-9	unrestricted	873	www.pubchem.com	4.40E-03	www.pubchem.com	224	www.pubchem.com	4.41	www.pubchem.com	107	Carl Roth GmbH + Co. KG	55.96	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
dioctyl ether	629-82-3	unrestricted	820	www.pubchem.com	1.00E-01	www.sigmaaldrich.com	300	www.pubchem.com	5.7	pubchem.ncbi.nlm.nih.gov	109	Deutsche Gesetzliche Un	83.64	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
2-phenylethyl 1-prop-1-en-2-ylcyclohexene	138-86-3	unrestricted	841	www.pubchem.com	1.38E-02	www.pubchem.com	176	www.pubchem.com	4.57	www.pubchem.com	43	Merck KGaA, Darmstadt,	5.12	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
dec-1-ene	872-05-9	unrestricted	741	www.pubchem.com	1.15E-04	www.pubchem.com	170.6	www.pubchem.com	5.7	www.pubchem.com	44	Deutsche Gesetzliche Un	20.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
decan-1-ol	112-30-1	unrestricted	829.7	www.pubchem.com	3.70E-02	www.pubchem.com	230	www.pubchem.com	4.57	www.pubchem.com	108	Deutsche Gesetzliche Un	21.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
dodec-1-ene	112-41-4	unrestricted	758	www.pubchem.com	0.00E+00	www.pubchem.com	212.8	www.pubchem.com	6.1	www.pubchem.com	77	Merck KGaA, Darmstadt,	24.10	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
dodecane	112-40-3	unrestricted	750	www.pubchem.com	3.70E-06	www.pubchem.com	216.3	www.pubchem.com	6.1	www.pubchem.com	70	Carl Roth GmbH + Co. KG	26.70	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
oct-1-ene	111-66-0	unrestricted	715	www.pubchem.com	4.10E-03	www.pubchem.com	172.1	www.pubchem.com	4.57	www.pubchem.com	8	Merck KGaA, Darmstadt,	29.10	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
octane	111-65-9	unrestricted	699	www.pubchem.com	6.60E-04	www.pubchem.com	126	www.pubchem.com	5.18	www.pubchem.com	13	Carl Roth GmbH + Co. KG	35.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
decane	124-18-5	unrestricted	730	www.pubchem.com	5.20E-05	www.pubchem.com	174.1	www.pubchem.com	5.01	www.pubchem.com	51	Merck KGaA, Darmstadt,	37.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
undecan-2-one	112-12-9	unrestricted	826	www.pubchem.com	2.00E-02	www.pubchem.com	231.5	www.pubchem.com	4.09	www.pubchem.com	96	Merck KGaA, Darmstadt,	38.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
nonane	111-84-2	unrestricted	718	www.pubchem.com	2.20E-04	www.pubchem.com	150.5	www.pubchem.com	5.65	www.pubchem.com	31	Merck KGaA, Darmstadt,	43.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
hexadecane	544-76-3	unrestricted	770	www.pubchem.com	9.00E-07	www.pubchem.com	287.2	www.pubchem.com	8.2	www.pubchem.com	135	Merck KGaA, Darmstadt,	54.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
undecane	1120-21-4	unrestricted	740	www.pubchem.com	4.40E-06	www.pubchem.com	195.5	www.pubchem.com	5.74	www.pubchem.com	56	Carl Roth GmbH + Co. KG	55.90	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
cyclooctane	292-64-8	unrestricted	834	www.sigmaaldrich.com	4.92E-03	www.chemspider.com	149	www.chemspider.com	4.45	www.chemspider.com	28	Merck KGaA, Darmstadt,	57.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
butylbenzene	104-51-8	unrestricted	860	www.pubchem.com	1.18E-02	www.pubchem.com	183.3	www.pubchem.com	4.38	www.pubchem.com	58	Merck KGaA, Darmstadt,	76.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
methyl nonanoate	1731-84-6	restricted	900	www.chemspider.com	2.29E-02	www.pubchem.com	213.5	www.pubchem.com	4.32	www.pubchem.com	87	Deutsche Gesetzliche Un	4.95	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
octyl acetate	112-14-1	restricted	868	www.chemspider.com	4.60E-02	www.chemspider.com	210	www.pubchem.com	3.81	www.chemspider.com	83	Deutsche Gesetzliche Un	31.25	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
(Z)-octadec-9-enoic acid	112-80-1	restricted	895	www.pubchem.com	1.15E-05	www.pubchem.com	286	www.pubchem.com	7.64	www.pubchem.com	189	Deutsche Gesetzliche Un	4.56	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1,2,4-trimethylbenzene	95-63-6	restricted	876	www.pubchem.com	5.70E-02	www.pubchem.com	168.9	www.pubchem.com	3.78	www.pubchem.com	50	Deutsche Gesetzliche Un	19.90	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2-methylpropane	98-82-8	restricted	862	www.pubchem.com	6.13E-02	www.pubchem.com	152.4	www.pubchem.com	3.66	www.pubchem.com	31	Deutsche Gesetzliche Un	20.90	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
nonan-1-ol	143-08-8	restricted	827	www.pubchem.com	1.40E-01	www.pubchem.com	213.3	www.pubchem.com	3.77	www.pubchem.com	98.5	Deutsche Gesetzliche Un	23.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
propylbenzene	103-65-1	restricted	862	www.pubchem.com	2.34E-02	www.pubchem.com	159	www.pubchem.com	3.69	www.pubchem.com	39	Deutsche Gesetzliche Un	26.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-chloroheptane	629-06-1	restricted	900	www.chemspider.com	2.52E-02	www.chemspider.com	159	www.pubchem.com	4.15	www.pubchem.com	38	www.chemspider.com	56.10	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2,2,4-trimethylpentane	540-84-1	restricted	692	www.pubchem.com	9.91E-03	www.chemspider.com	99.2	www.pubchem.com	4.46	www.chemspider.com	-9	Deutsche Gesetzliche Un	60.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
heptane	142-82-5	restricted	680	www.pubchem.com	3.40E-03	www.pubchem.com	98.4	www.pubchem.com	4.66	www.pubchem.com	-7	Deutsche Gesetzliche Un	63.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
(1Z,5Z)-cycloocta-1,5-diene	111-78-4	restricted	882	www.pubchem.com	0.00E+00	www.pubchem.com	150.8	www.pubchem.com	3.67	www.chemspider.com	31	Deutsche Gesetzliche Un	70.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
methylcyclohexane	108-87-2	restricted	770	www.pubchem.com	1.40E-02	www.pubchem.com	100.9	www.pubchem.com	3.61	www.pubchem.com	4	Deutsche Gesetzliche Un	79.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2-ethylhexyl 2-methylprop-2-enoate	688-84-6	restricted	880	www.pubchem.com	5.92E-03	www.chemspider.com	110	www.pubchem.com	4.54	www.pubchem.com	92	Merck KGaA, Darmstadt,	106.80	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
bis(2-methyloctyl) benzene-1,2-dicarboxylate	68515-48-0	not suitable	990	www.chemspider.com	2.32E-08	www.chemspider.com	405	www.chemspider.com	9.77	www.chemspider.com	216.3	www.chemspider.com	4.14	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
bis(2-ethylhexyl) benzene-1,4-dicarboxylate	6422-86-2	not suitable	900	www.chemspider.com	2.39E-07	www.chemspider.com	400	www.sigmaaldrich.com	9.55	www.chemspider.com	212	Merck KGaA, Darmstadt,	4.97	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
2-ethylhexyl 3-methylbutanoate	140-25-1	not suitable	1000	www.chemspider.com	1.05E-02	www.chemspider.com	268	www.chemspider.com	3.81	www.chemspider.com	113	Merck KGaA, Darmstadt,	10.92	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
benzylbenzene	101-81-5	not suitable	1010	www.chemspider.com	1.83E-02	www.chemspider.com	262	www.chemspider.com	4.21	www.chemspider.com	120	www.chemspider.com	10.92	www.sigmaaldrich.com	24.05.2020	1	https://echa.europa.eu/information-on-chemicals
Butyl benzoate	136-60-7	not suitable	1010	www.chemspider.com	2.95E-02	www.chemspider.com	249	www.sigmaaldrich.com	3.79	www.chemspider.com							

Benzyl benzoate	120-51-4	not suitable	1120	www.chemspider.com	1.54E-02	www.chemspider.com	324	www.sigmaaldrich.com	3.97	www.pubchem.com	158	Merck KGaA, Darmstadt,	20.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
Octanal	124-13-0	not suitable	820	www.chemspider.com	3.94E-01	www.chemspider.com	271	www.sigmaaldrich.com	3.07	www.chemspider.com	52	Merck KGaA, Darmstadt,	20.80	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
benzyl 2-methylprop-2-enoate	2495-37-6	not suitable	1040	www.chemspider.com	3.97E-01	www.chemspider.com	131	www.sigmaaldrich.com	2.82	www.chemspider.com	107	Merck KGaA, Darmstadt,	21.24	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
Ethylbenzene	100-41-4	not suitable	867	www.pubchem.com	1.70E-01	www.pubchem.com	1362	www.pubchem.com	3.15	pubchem.ncbi.nlm.nih.gov	15	www.pubchem.com	21.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
Anisole	100-66-3	not suitable	990	www.chemspider.com	1.74E+00	www.chemspider.com	194	www.sigmaaldrich.com	2.13	www.chemspider.com	43	Merck KGaA, Darmstadt,	21.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
phenoxybenzene	101-84-8	not suitable	1070	www.chemspider.com	1.56E-02	www.chemspider.com	258	www.pubchem.com	4.21	www.chemspider.com	115	www.pubchem.com	22.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-bromohexane	111-25-1	not suitable	1180	www.chemspider.com	3.69E-02	www.chemspider.com	1553	www.chemspider.com	3.81	www.chemspider.com	47	Merck KGaA, Darmstadt,	23.10	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2,6-diethylaniline	579-66-8	not suitable	960	www.pubchem.com	6.70E-01	www.pubchem.com	2355	www.pubchem.com	0.95	www.pubchem.com	115	Merck KGaA, Darmstadt,	23.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-bromohexane	629-04-9	not suitable	1140	www.chemspider.com	1.05E-02	www.chemspider.com	179	www.pubchem.com	4.34	www.chemspider.com	60	Merck KGaA, Darmstadt,	23.26	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-bromodecane	112-29-8	not suitable	1070	www.chemspider.com	5.65E-04	www.chemspider.com	2406	www.pubchem.com	5.93	www.chemspider.com	94	Merck KGaA, Darmstadt,	23.43	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1H-indene	95-13-6	not suitable	996	www.chemspider.com	0.3324	www.chemspider.com	182	www.pubchem.com	2.91	www.chemspider.com	58	Merck KGaA, Darmstadt,	26.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
bromomethylbenzene	100-39-0	not suitable	1440	www.chemspider.com	1.95E-01	www.chemspider.com	198	www.pubchem.com	2.91	www.chemspider.com	87	www.chemspider.com	30.20	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1,2-xylylene	95-47-6	not suitable	880	www.chemspider.com	0.2424	www.chemspider.com	144	www.pubchem.com	3.14	www.chemspider.com	30	Merck KGaA, Darmstadt,	31.60	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-bromopentane	110-53-2	not suitable	1220	www.chemspider.com	9.94E-02	www.chemspider.com	130	www.sigmaaldrich.com	3.27	www.chemspider.com	82	Merck KGaA, Darmstadt,	34.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
Cyclopentane	287-92-3	not suitable	750	www.chemspider.com	1.08E-01	www.chemspider.com	50	www.sigmaaldrich.com	2.82	www.chemspider.com	-20	Merck KGaA, Darmstadt,	38.30	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2,3-dihydro-1H-indene	496-11-7	not suitable	960	www.chemspider.com	1.96E-01	www.chemspider.com	176	www.sigmaaldrich.com	3.34	www.chemspider.com	54	Merck KGaA, Darmstadt,	46.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-chloro-4-methylbenzene	106-43-4	not suitable	1070	www.pubchem.com	1.06E-01	www.pubchem.com	162	www.pubchem.com	3.33	www.pubchem.com	51	Merck KGaA, Darmstadt,	51.47	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
cyclohexyl 2-methylprop-2-enoate	101-43-9	not suitable	970	www.chemspider.com	1.33E-01	www.chemspider.com	210	www.chemspider.com	3.4	www.chemspider.com	78	www.chemspider.com	54.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
Cyclopentyl methyl ether	5614-37-9	not suitable	860	www.chemspider.com	3.10E+00	www.chemspider.com	1053	www.chemspider.com	1.59	pubchem.ncbi.nlm.nih.gov	-1	Merck KGaA, Darmstadt,	55.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-chloro-3-methylbenzene	108-41-8	not suitable	1072	www.pubchem.com	1.50E-01	www.pubchem.com	1622	www.chemspider.com	3.27	www.chemspider.com	52	Merck KGaA, Darmstadt,	55.74	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-iodoheptane	4282-40-0	not suitable	1380	www.chemspider.com	3.09E-03	www.chemspider.com	204	www.pubchem.com	4.7	www.pubchem.com	76	Merck KGaA, Darmstadt,	65.41	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1,3-xylylene	128-38-3	not suitable	870	www.chemspider.com	2.07E-01	www.chemspider.com	138	www.sigmaaldrich.com	3.14	www.chemspider.com	25	Merck KGaA, Darmstadt,	85.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
iodobenzene	108-91-5	not suitable	180	www.chemspider.com	7.00E-02	www.chemspider.com	188	www.chemspider.com	2.97	www.chemspider.com	77	Merck KGaA, Darmstadt,	85.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-methoxy-3-methylbenzene	100-84-5	not suitable	970	www.chemspider.com	0.00E+00	www.chemspider.com	1755	www.pubchem.com	2.59	www.chemspider.com	54	www.chemspider.com	91.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
phenylsulfanybenzene	139-66-2	not suitable	1110	www.chemspider.com	8.12E-03	www.chemspider.com	296	www.chemspider.com	4.45	www.chemspider.com	110	Merck KGaA, Darmstadt,	100.90	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-methoxy-2-methylbenzene	578-58-5	not suitable	990	www.chemspider.com	4.50E-01	www.chemspider.com	171	www.pubchem.com	2.74	www.pubchem.com	52	Merck KGaA, Darmstadt,	108.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
octan-3-ol	589-98-0	not suitable	820	www.chemspider.com	1.38E+00	www.chemspider.com	169	www.chemspider.com	2.73	www.chemspider.com	68	Merck KGaA, Darmstadt,	110.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
N-butylaniline	1126-78-9	not suitable	930	www.chemspider.com	6.70E-02	www.chemspider.com	236	www.sigmaaldrich.com	3.19	www.chemspider.com	106	Merck KGaA, Darmstadt,	122.76	www.vwr.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
hexylbenzene	1077-16-3	not suitable	860	www.chemspider.com	1.29E-03	www.chemspider.com	2261	www.chemspider.com	5.52	www.chemspider.com	83	Merck KGaA, Darmstadt,	152.22	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
prop-2-enylbenzene	300-57-2	not suitable	890	www.chemspider.com	1.78E-01	www.chemspider.com	156	www.sigmaaldrich.com	3.24	www.chemspider.com	40	Merck KGaA, Darmstadt,	155.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
hept-1-ene	592-76-7	not suitable	697	www.pubchem.com	1.82E-02	www.pubchem.com	936	www.pubchem.com	3.99	www.pubchem.com	-8	Deutsche Gesetzliche Un	170.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-ethyl-4-methylbenzene	622-96-8	not suitable	860	www.chemspider.com	7.96E-02	www.chemspider.com	162	www.pubchem.com	3.63	www.pubchem.com	43	www.chemspider.com	175.44	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2-methoxy-2-methylbutane	994-05-8	not suitable	766	www.chemspider.com	0.7	www.chemspider.com	863	www.pubchem.com	1.55	pubchem.ncbi.nlm.nih.gov	-7	Merck KGaA, Darmstadt,	187.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
prop-2-enylbenzene	1746-13-0	not suitable	980	www.chemspider.com	0.00E+00	www.chemspider.com	192	www.sigmaaldrich.com	2.06	www.chemspider.com	63	Merck KGaA, Darmstadt,	217.56	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1,2,3-trimethylbenzene	526-73-8	not suitable	894	www.pubchem.com	7.52E-02	www.pubchem.com	176	www.pubchem.com	3.66	www.pubchem.com	51	Deutsche Gesetzliche Un	230.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1-benzothioephene	95-15-8	not suitable	1150	www.chemspider.com	0.1916	www.chemspider.com	221	www.sigmaaldrich.com	4.38	www.chemspider.com	91	www.chemspider.com	241.50	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
decylbenzene	104-72-3	not suitable	855	www.chemspider.com	1.10E-08	www.pubchem.com	298	www.pubchem.com	7.37	www.pubchem.com	110	www.chemspider.com	351.41	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
N-methyl-N-phenylaniline	552-82-9	not suitable	1050	www.chemspider.com	2.48E-02	www.chemspider.com	180	www.sigmaaldrich.com	3.9	www.chemspider.com	110	Merck KGaA, Darmstadt,	567.00	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
non-1-ene	124-11-8	not suitable	743	www.pubchem.com	1.12E-03	www.pubchem.com	1469	www.pubchem.com	5.15	www.pubchem.com	24	Merck KGaA, Darmstadt,	594.68	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
1,2,3,4-tetramethylbenzene	488-23-3	not suitable	900	www.chemspider.com	3.39E-02	www.chemspider.com	205	www.pubchem.com	4	www.pubchem.com	68	www.chemspider.com	738.09	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
propan-2-yl benzoate	939-48-0	not suitable	1000	www.chemspider.com	0.126	www.chemspider.com	216	www.pubchem.com	3.08	www.chemspider.com	99	www.chemspider.com	918.40	www.sigmaaldrich.com	24.05.2020	2	https://echa.europa.eu/information-on-chemicals
4-butyropyridine	5335-75-1	not suitable	900	www.chemspider.com	3.71E+00	www.chemspider.com	209	www.pubchem.com	2.78	www.chemspider.com	74.6	www.chemspider.com	n.a.		24.05.2020	2	Merck KGaA, Darmstadt, Germany
octan-4-ol	589-62-8	not suitable	900	www.chemspider.com	1.53E+00	www.chemspider.com	174	www.sigmaaldrich.com	2.82	www.chemspider.com	65	Merck KGaA, Darmstadt,	n.a.		24.05.2020	2	https://echa.europa.eu/information-on-chemicals
2,2-Dimethylpropane	463-82-1	not suitable	610	www.chemspider.com	8.63E-02	www.chemspider.com	95	www.sigmaaldrich.com	3.05	www.chemspider.com	-17.15	www.chemspider.com	n.a.		24.05.2020	2	https://echa.europa.eu/information-on-chemicals
propylbenzene	623-8																

cyclododeca-1,5,9-triene	706-31-0	not suitable	880 www.chemspider.com	4.70E-04 www.pubchem.com	231 www.pubchem.com	5.5 www.pubchem.com	88 www.pubchem.com	n.a.	24.05.2020	6 https://echa.europa.eu/information-on-chemicals
1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene	91-17-8	not suitable	890 www.pubchem.com	8.89E-04 www.pubchem.com	195 www.pubchem.com	4.93 www.chemspider.com	56 Deutsche Gesetzliche Un	10.12 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
octan-1-amine	111-86-4	not suitable	780 www.chemspider.com	3.15E+00 www.chemspider.com	178 www.sigmaaldrich.com	3.06 www.chemspider.com	58 Merck KGaA, Darmstadt,	15.20 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
Hexane	110-54-3	not suitable	660 www.chemspider.com	1.72E-02 www.chemspider.com	68.73 www.pubchem.com	3.94 www.chemspider.com	-26 Merck KGaA, Darmstadt,	24.60 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
Chloroform	67-66-3	not suitable	1490 www.chemspider.com	2.10E+00 www.chemspider.com	61.1 www.pubchem.com	1.75 www.chemspider.com	n.a. www.pubchem.com	34.00 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
Octanoic acid	124-07-2	not suitable	910 www.chemspider.com	4.96E-01 www.chemspider.com	237 www.sigmaaldrich.com	2.9 www.chemspider.com	110 Merck KGaA, Darmstadt,	50.30 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
2,3-dimethylbutane	79-29-8	not suitable	662 www.pubchem.com	2.25E-02 www.pubchem.com	57.9 www.pubchem.com	3.42 www.pubchem.com	-29 Merck KGaA, Darmstadt,	66.40 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
tetrachloromethane	56-23-5	not suitable	1590 www.chemspider.com	2.80E-01 www.chemspider.com	76 www.sigmaaldrich.com	2.86 www.chemspider.com	-0.3 www.chemspider.com	193.00 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
decan-1-amine	2016-57-1	not suitable	730 www.pubchem.com	4.23E-01 www.chemspider.com	220.5 www.pubchem.com	1.92 www.pubchem.com	89 Merck KGaA, Darmstadt,	252.58 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
nonan-1-amine	112-20-9	not suitable	780 www.chemspider.com	1.28E+00 www.chemspider.com	202 www.sigmaaldrich.com	3.59 www.chemspider.com	63 Merck KGaA, Darmstadt,	393.60 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
2,2-dimethylbutane	75-83-2	not suitable	644 www.pubchem.com	2.12E-02 www.pubchem.com	49.7 www.pubchem.com	3.82 www.pubchem.com	-29 Merck KGaA, Darmstadt,	881.00 www.sigmaaldrich.com	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
4-Propylphenol	645-56-7	not suitable	980 www.chemspider.com	6.11E-01 www.chemspider.com	232 www.sigmaaldrich.com	3.01 www.chemspider.com	106 Merck KGaA, Darmstadt,	n.a.	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
4-butylphenol	1638-22-8	not suitable	980 www.chemspider.com	2.20E-01 www.chemspider.com	248 www.pubchem.com	3.54 www.chemspider.com	22 www.chemspider.com	n.a.	24.05.2020	7 https://echa.europa.eu/information-on-chemicals
dibutyl benzene-1,2-dicarboxylate	84-74-2	not suitable	1050 www.chemspider.com	0.00235 www.chemspider.com	340 www.sigmaaldrich.com	4.82 www.chemspider.com	171 Merck KGaA, Darmstadt,	26.10 www.sigmaaldrich.com	24.05.2020	9 https://echa.europa.eu/information-on-chemicals
1,1,2-trichloroethane	79-00-5	not suitable	1442 www.pubchem.com	4.50E-03 www.pubchem.com	114 www.pubchem.com	1.89 www.pubchem.com	114 www.chemspider.com	26.76 www.sigmaaldrich.com	24.05.2020	9 https://echa.europa.eu/information-on-chemicals
bis(2-ethylhexyl) benzene-1,2-dicarboxylate	117-81-7	not suitable	990 www.pubchem.com	2.70E-04 www.pubchem.com	384 www.pubchem.com	7.6 www.pubchem.com	207 Merck KGaA, Darmstadt,	n.a.	24.05.2020	9 https://echa.europa.eu/information-on-chemicals
Benzene	71-43-2	not suitable	879 www.pubchem.com	1.79E+00 www.pubchem.com	80 www.pubchem.com	2.13 pubchem.ncbi.nlm.nih.gov	-11 Merck KGaA, Darmstadt,	48.70 www.sigmaaldrich.com	24.05.2020	10 https://echa.europa.eu/information-on-chemicals