

Compounds known not to be contact allergens.

For toxicity and effect values, consult TerraTox™ databases, or TerraBase Inc.

CAS	EINECS	RTECS	Name	SMILES	Formula	MW
461-58-5	207-312-8	ME 9950000	2-cyanoguanidine; dicyanodiamide	<chem>NC(=NC(#N))N</chem>	C2H4N4	84.08
79-14-1	201-180-5	MC 5250000	glycolic acid	<chem>O=C(O)CO</chem>	C2H4O3	76.05
96-26-4	202-494-5	UC 1645000	dihydroxyacetone	<chem>OCC(=O)CO</chem>	C3H6O3	90.08
6898-95-9	-	-	L-serine	<chem>OC[C@H](N)C(=O)O</chem>	C3H7NO3	105.09
57-55-6	200-338-0	TY 2000000	1,2-propanediol, DL; propylene glycol	<chem>OCC(O)C</chem>	C3H8O2	76.10
56-81-5	200-289-5	MA 8050000	1,2,3-propanetriol; glycerol	<chem>OCC(O)CO</chem>	C3H8O3	92.09
97-59-6	202-592-8	YT 1600000	allantoin	<chem>O=C(NC(NC(=O)N1)C1=O)N</chem>	C4H6N4O3	158.12
51200-87-4	257-048-2	RP 7211000	4,4-dimethylloxazolidine	<chem>O1CNC(C)(C)C1</chem>	C5H11NO	101.15
118-71-8	204-271-8	UQ 1050000	maltol	<chem>O1C(C)=C(O)C(=O)C=C1</chem>	C6H6O3	126.11
61-90-5	200-522-0	OH 2850000	leucine, L	<chem>O=C(O)C(N)CC(C)C</chem>	C6H13NO2	131.17
65-85-0	200-618-2	DG 0875000	benzoic acid	<chem>O=C(O)c(cccc1)c1</chem>	C7H6O2	122.12
69-72-7	200-712-3	VO 0525000	2-hydroxybenzoic acid; salicylic acid	<chem>O=C(O)c(c(O)ccc1)c1</chem>	C7H6O3	138.12
58-55-9	200-385-7	XH 3850000	xanthine, 1,3-dimethyl; theophylline	<chem>CN1C(=O)N(C)c2ncnc2C1(=O)</chem>	C7H8N4O2	180.17
100-66-3	202-876-1	BZ 8050000	anisole	<chem>O(c(cccc1)c1)C</chem>	C7H8O	108.14
103-64-0	203-131-3	WL 3850000	1-bromo-2-phenylethylene	<chem>Br/C=C/c1ccccc1</chem>	C8H7Br	183.05
120-72-9	204-420-7	NL 2450000	indole	<chem>c1ccc2ccnc2c1</chem>	C8H7N	117.15
100-42-5	202-851-5	WL 3675000	styrene	<chem>c(cccc1)(c1)C=C</chem>	C8H8	104.15
123-11-5	204-602-6	BZ 2625000	4-methoxybenzaldehyde; anisic aldehyde	<chem>O=Cc(ccc(OC)c1)c1</chem>	C8H8O2	136.15
119-36-8	204-317-7	VO 4725000	methyl salicylate	<chem>O=C(OC)c(c(O)ccc1)c1</chem>	C8H8O3	152.15
134-20-3	205-132-4	CB 3325000	methyl 2-aminobenzoate; methyl anthranilate	<chem>O=C(OC)c(c(N)ccc1)c1</chem>	C8H9NO2	151.16
58-08-2	200-362-1	EV 6475000	xanthine, 1,3,7-trimethyl; caffeine	<chem>CN1C(=O)N(C)c2ncn(C)c2C1(=O)</chem>	C8H10N4O2	194.19
60-12-8	200-456-2	SG 7175000	2-phenylethanol	<chem>OCCc(cccc1)c1</chem>	C8H10O	122.17
95-65-8	202-439-5	ZE 6300000	3,4-dimethylphenol	<chem>Oc(ccc(c1C)C)c1</chem>	C8H10O	122.17
98-85-1	202-707-1	DO 9275000	1-phenylethanol	<chem>OC(c(cccc1)c1)C</chem>	C8H10O	122.17
105-13-5	203-273-6	DO 8925000	4-methoxybenzyl alcohol; anisyl alcohol	<chem>O(c(ccc(c1)CO)c1)C</chem>	C8H10O2	138.17
617-73-2	210-524-3	-	2-hydroxy-n-octanoic acid; alpha-hydroxycaprylic acid	<chem>CCCCCCC(O)C(=O)O</chem>	C8H16O3	160.21
22457-23-4	245-010-8	MJ 7430000	5-methyl-3-heptanone oxime	<chem>CC/C(=N/O)CC(C)CC</chem>	C8H17NO	143.23
91-64-5	202-086-7	GN 4200000	coumarin	<chem>c1cc2OC(=O)C=Cc2cc1</chem>	C9H6O2	146.15
119-65-3	204-341-8	NW 6825000	isoquinoline	<chem>n(ccc(c1ccc2)c2)c1</chem>	C9H7N	129.16
140-10-3	205-398-1	GD 7800000	trans-cinnamic acid	<chem>O=C(O)/C=C/c(cccc1)c1</chem>	C9H8O2	148.16
104-53-0	203-211-8	MW 4890000	benzenepropanal; 3-phenylpropionaldehyde	<chem>c1ccccc1CCC=O</chem>	C9H10O	134.18
100-06-1	202-815-9	AM 2400000	4'-methoxyacetophenone	<chem>O=C(c(ccc(OC)c1)c1)C</chem>	C9H10O2	150.18
140-39-6	205-413-1	AJ 7570000	p-tolyl acetate	<chem>O=C(Oc(ccc(c1)C)c1)C</chem>	C9H10O2	150.18
60-18-4	200-460-4	YP 2275600	tyrosine, L	<chem>O=C(O)C(N)Cc(ccc(O)c1)c1</chem>	C9H11NO3	181.19
98-82-8	202-704-5	GR 8575000	isopropylbenzene; cumene	<chem>c(cccc1)(c1)C(C)C</chem>	C9H12	120.19
80-39-7	-	-	N-ethyl 4-toluenesulfonamide	<chem>O=S(=O)(NCC)c(ccc(c1)C)c1</chem>	C9H13NO2S	199.27
68039-48-5	268-263-6	-	3,5-dimethylcyclohex-3-en-1-yl carboxaldehyde	<chem>C1C(C)C=C(C)CC1C=O</chem>	C9H14O	138.21
104-61-0	203-219-1	LU 3675000	gamma-nonalactone	<chem>O=C(OC(C1)CCCC)C1</chem>	C9H16O2	156.23
124-19-6	204-688-5	RA 5700000	nonanal	<chem>O=CCCCCCCC</chem>	C9H18O	142.24
16485-10-2	-	ES 4316500	panthenol (R/S)	<chem>OC(C(=O)NCCCO)C(C)(C)CO</chem>	C9H19NO4	205.25
581-43-1	209-465-6	-	2,6-dihydroxynaphthalene	<chem>Oc(ccc(c1ccc2O)c2)c1</chem>	C10H8O2	160.17
1459-93-4	215-951-9	NT 2540000	dimethyl isophthalate	<chem>O=C(OC)c(cccc1C(=O)OC)c1</chem>	C10H10O4	194.19
50770-19-9	-	-	1-(4-methoxyphenyl)propene	<chem>c1cc(OC)ccc1/C=C/C</chem>	C10H12O	148.20
104-21-2	203-185-8	-	4-methoxybenzyl acetate	<chem>c1cc(OC)ccc1COC(=O)C</chem>	C10H12O3	180.20

T-4735-004	-		alpha-glyceryl 4-aminobenzoate	<chem>OCC(O)COC(=O)c1ccc(N)cc1</chem>	C10H13NO4	211.22
54-11-5	200-193-3	QS 5250000	nicotine S(-)	<chem>n(cccc1[C@H](N(CC2)C)C2)c1</chem>	C10H14N2	162.23
100-86-7	202-896-0	SG 8050000	2-methyl-1-phenyl-2-propanol	<chem>c1ccccc1CC(C)(O)C</chem>	C10H14O	150.22
89-83-8	201-944-8	XP 2275000	2-isopropyl-5-methylphenol; thymol	<chem>Oc(c(ccc1C)C(C)C)c1</chem>	C10H14O	150.22
3338-55-4	222-081-3	-	3,7-dimethyl -1,3,6-octatriene (3Z)	<chem>C=C/C(C)=C\C/C=C(C)/C</chem>	C10H16	136.24
76-22-2	200-945-0	EX 1225000	camphor; see also CAS 21368-68-3	<chem>O=C(C(C(C1C2)(C)C)(C2)C)C1</chem>	C10H16O	152.24
106-25-2	203-378-7	RG 5840000	nerol; 3,7-dimethyl-2,6-octadiene-1-ol (Z); 2-cis-3,7-dimethyl-2,6-octadien-1-ol	<chem>OC/C([H])=C(C)\CC/C=C(C)/C</chem>	C10H18O	154.25
78-70-6	201-134-4	RG 5775000	linalool; 3,7-dimethylocta-1,6-dien-3-ol	<chem>C/C(C)=C/CCC(C)(O)C=C</chem>	C10H18O	154.25
111-79-5	203-908-7	RA 9470000	methyl 2-nonenoate	<chem>CCCCCC/C=C/C(=O)OC</chem>	C10H18O2	170.25
89-78-1	201-939-0	OT 0350000	(±)-menthol	<chem>OC(C(CCC1C)C(C)C)C1</chem>	C10H20O	156.27
112-45-8	203-973-1	YQ 2835000	10-undecen-1-al; undecylenic aldehyde	<chem>O=CCCCCCCCC=C</chem>	C11H20O	168.28
104-67-6	203-225-4	YQ 2485000	gamma-undecalactone	<chem>O=C(OC(C1)CCCCC)C1</chem>	C11H20O2	184.28
112-43-6	203-971-0	YQ 2985000	10-undecen-1-ol	<chem>OCCCCCCCCC=C</chem>	C11H22O	170.29
93-08-3	202-216-2	AL 2988000	2-acetonaphthone	<chem>O=C(c(ccc(c1ccc2)c2)c1)C</chem>	C12H10O	170.21
135-79-5	205-220-2	-	6-isopropylquinoline	<chem>c1c(C(C)C)ccc2c1cccn2</chem>	C12H13N	171.24
93-29-8	202-236-1	SL 7940000	2-methoxy-4-(propen-1-yl)phenyl acetate	<chem>COc1cc(/C=C/C)ccc1OC(=O)C</chem>	C12H14O3	206.24
84-66-2	201-550-6	TI 1050000	diethyl phthalate; DEP	<chem>O=C(OCC)c(c(ccc1)C(=O)OCC)c1</chem>	C12H14O4	222.24
81-15-2	201-329-4	CZ 7210000	nitromusk xylene; 1-tert-butyl-3,5-dimethyl-2,4,6-trinitrobenzene	<chem>O=N(=O)c1c(c(c(c1C)N(=O)=O)C(C)C)N(=O)=O)C</chem>	C12H15N3O6	297.27
83-66-9	201-493-7	BZ 8575000	nitromusk ambrette; 1-tert-butyl-3,5-dinitro-2-methoxy-4-methylbenzene	<chem>O=N(=O)c(c(c(N(=O)=O)c(OC)c1C(C)C)C)C1</chem>	C12H16N2O5	268.27
151-05-3	205-781-3	SG 8100000	alpha, alpha-dimethylphenylethyl acetate; dimethylbenzylcarbiny acetate; 2-benzyl-2-propyl acetate	<chem>c1ccccc1CC(C)(C)OC(=O)C</chem>	C12H16O2	192.26
97-23-4	202-567-1	SM 0175000	dichlorophen; 5,5'-dichloro-2,2'-dihydroxydiphenylmethane; Panacide	<chem>Clc1ccc(O)c(c1)C2cc(Cl)ccc2O</chem>	C13H10Cl2O2	269.13
93-19-6	202-227-2	VC 0245000	2-isobutylquinoline	<chem>n1c(CC(C)C)ccc2ccccc12</chem>	C13H15N	185.27
57754-81-1	-	-	n-butyl 4-dimethylaminobenzoate	<chem>c1cc(N(C)C)ccc1C(=O)OCCCC</chem>	C13H19NO2	221.30
50-29-3	200-024-3	KJ 3325000	DDT, p,p'-; X= Cl, Y= Cl, Z= Cl	<chem>c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl</chem>	C14H9Cl5	354.49
103-30-0	203-098-5	WJ 4926500	trans-stilbene	<chem>c(cccc1)(c1)/C=C/c(cccc2)c2</chem>	C14H12	180.25
131-57-7	205-031-5	DJ 1575000	2-hydroxy-4-methoxybenzophenone; Eusolex 4360; HMB; Oxybenzone	<chem>O=C(c(cccc1)c1)c(c(O)cc(OC)c2)c2</chem>	C14H12O3	228.25
81-14-1	201-328-9	-	nitromusk ketone; 4-tert-butyl-2,6-dimethyl-3,5-dinitroacetophenone	<chem>O=C(c1c(c(c(c1C)N(=O)=O)C(C)C)N(=O)=O)C</chem>	C14H18N2O5	294.31
1117-41-5	YQ 2833800		isomethylionone; 2,6,9-trimethylundeca-2,6,8-trien-10-one [isomer mixture]; 3,6,10-trimethyl-3,5,9-undecatriene-2-one	<chem>CC(=O)/C(C)=C/C=C(C)/CC/C=C(C)/C</chem>	C14H22O	206.33
6969-49-9	230-190-2	VO 5400000	n-octyl salicylate	<chem>Oc1ccccc1C(=O)OCCCCCCCC</chem>	C15H22O3	250.34

142-18-7	205-526-6	OF 1600000	1-monomyristin; alpha-glyceryl laurate; (+)-glyceryl 1-monododecanoate	OCC(O)COC(=O)CCCCCCCCCCC	C15H30O4	274.40
89-46-3	201-909-7	-	benzoic acid, 2-hydroxy-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, (1alpha,2beta,5alpha)-; menthyl salicylate	O=C(OC(C(CCC1C)C(C)C)C1)c(O)ccc2c2	C17H24O3	276.38
50-28-2	200-023-8	KG 2975000	17beta-estradiol, (+)	c1c(O)ccc2[C@@]3([H])CC[C@]4(C)[C@](O)([H])CC[C@@]4([H])[C@]3([H])CCc12	C18H24O2	272.39
88-29-9		AL 3031000	versalide; 1,1,4,4-tetramethyl-6-ethyl-7-acetyltetralin	c1c(CC)c(C(=O)C)cc2C(C)(C)CCC(C)(C)c12	C18H26O	258.40
28645-51-4	249-120-7	-	9-hexadecenolide; oxacycloheptadec-10-en-2-one; ambrettolide	C1CCCCCCCC/C=C/CCCCCOC1=O	C18H32O2	280.45
58-22-0		XA 3030000	testosterone	O=C1CC[C@]2(C)[C@@]3([H])CC[C@@]4(C)[C@](O)([H])CC[C@@]4([H])C3CCC2=C1	C19H28O2	288.43
514-10-3	208-178-3	TP 8580000	abietic acid	O=C(O)[C@@]([C@@]([H])([C@@](C(C(=C1)C=C(C2)C(C)C2)(CC3)C)C1)(C3)C	C20H30O2	302.46
506-32-1		CE 6675000	arachidonic acid; 5,8,11,14-eicosatetraenoic acid (5Z,8Z,11Z,14Z)	OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC	C20H32O2	304.47
24909-91-9		-	pregnane	C1CCC[C@]2(C)[C@@]3([H])CC[C@@]4(C)[C@](CC)([H])CC[C@@]4([H])[C@]3([H])CCC12	C21H36	288.52
105-97-5		-	di-n-decyl adipate; hexane-1,6-dioic acid, di-n-decyl ester	CCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCC	C26H50O4	426.68
57-88-5	200-353-2	FZ 8400000	cholesterol; cholest-5-en-3beta-ol	[C@@]12(C)C3CC[C@]4(C)[C@@]([H])([C@]([H])(C)CCCC(C)C)CCC4C3CC=C1C[C@](O)([H])CC2	C27H46O	386.66
59-02-9		DJ 2900000	Vitamin E; see also CAS 10191-41-0	O(c(c(c(c(O)c1C)C)CC2)c1C)C2(CC(CC(C)C)C)C	C29H50O2	430.72
7235-40-7	230-636-6	FI 0329500	trans-beta-carotene	CC1=C(C(C)(C)CCC1)/C=C/C(C)=C/C=C(C)=C/C=C(C)=C/C=C(C)=C/C=C(C)C	C40H56	536.88
T-4735-005		-	Ambersage	unavailable	unavailable	unavailable

You may freely use this material, but you must acknowledge its source in any publication resulting from its use.
 Copyright © 2005, TerraBase Inc.