

**Table 10a.** List of ketones in human body.

CAS-number	Compound name	Formula	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva	Semen
<i>Aliphatic straight chain</i>										
67-64-1	acetone / 2-propanone	C <sub>3</sub> H <sub>6</sub> O	[9, 216, 222, 223, 247, 248]	[193, 194, 196, 197, 202, 250, 252, 255-258]	[6, 55-57, 59, 60, 87, 106, 134, 259, 263, 264, 265, 268, 273-275, 278, 279, 281, 284, 286-288, 290, 293, 296, 298, 299, 301, 307-309, 311, 312, 315-320, 322, 324, 326, 329, 330, 335, 338, 340, 345, 347, 350, 357, 358, 361, 363, 364, 367-372, 377, 378, 380, 381, 385, 389, 390, 393, 394, 404-407]	[176, 191, 410]	[155, 163]	[122, 123, 131, 134, 138, 141, 417]	[110, 115, 418, 423]	[241]

78-93-3	butanone / 2-butanone / methyl ethyl ketone / MEK	C4H8O	[9, 216, 222, 223, 247, 248]	[193, 194, 196, 198, 202, 250, 255-258]	[6, 56, 57, 106, 259, 271, 275, 276, 286, 295, 303, 310, 311, 313, 332, 334, 336, 338, 351, 364, 368, 370, 372, 378, 393, 404, 406]	[178, 410]	[155, 163]	[106, 123, 125, 127, 138, 141]	[110, 111, 113, 115]	[241]
ui	pentanone	C5H10O							[114]	
96-22-0	3-pentanone	C5H10O	[9, 222]	[194, 258]	[277]	[178]		[123]		
107-87-9	2-pentanone / methyl propyl ketone	C5H10O	[9, 216, 222, 223, 247, 248]	[193, 194, 196, 198, 202, 250, 251, 254-258]	[6, 56, 57, 106, 259, 275, 277, 303, 305, 310, 311, 332, 364, 389, 406]	[178, 191, 410]	[155, 163]	[106, 125, 126]	[110, 115, 116]	[241]
591-78-6	2-hexanone	C6H12O	[9, 216, 222, 223, 247, 248,]	[194, 196, 254, 256, 258]	[6, 275, 305, 341]	[178, 410]		[106]		
589-38-8	3-hexanone	C6H12O	[9]	[193, 194, 196, 250, 254-258]	[6, 378]			[106, 124]	[111]	
123-19-3	4-heptanone	C7H14O	[9]	[193, 194, 196, 198, 202, 250, 253-258]	[6, 106, 275]		[155]	[106, 124]	[110, 115]	[241]

110-43-0	2-heptanone	C7H14O	[9, 216, 223, 247, 248]	[193, 194, 196, 202, 250, 253, 255-258]	[6, 106, 305, 324, 331]	[410]	[155, 156, 167]	[106, 124]	[110, 111]	[241]
106-35-4	3-heptanone	C7H14O	[9]	[194, 196, 250, 256-258]	[364, 408]		[155, 167]			[241]
589-63-9	4-octanone	C8H16O		[196, 202, 256, 258]				[128, 416]		
27457-18-7	octanone ui	C8H16O					[155]			
111-13-7	2-octanone	C8H16O	[9, 247]	[194, 256, 258]	[408]	[409]			[110, 111]	
106-68-3	3-octanone	C8H16O	[9]	[196, 255, 256, 258]	[408]		[156, 163]	[124]	[110]	
925-78-0	3-Nonanone	C9H18O					[167]			
821-55-6	2-nonanone	C9H18O	[9, 247]	[194, 196, 253, 255, 256, 258]	[408]	[182]	[155, 156]	[124, 125]	[110, 111]	
4485-09-0	4-nonanone	C9H18O		[194]						
693-54-9	2-decanone	C10H20O	[9, 247]			[178, 192]	[155]		[110, 111, 420]	
112-12-9	2-undecanone	C11H22O	[9, 247]	[253]		[182]	[156]	[124]	[110, 111, 420]	
2216-87-7	3-undecanone	C11H22O						[125]		
6064-27-3	6-dodecanone	C12H24O							[118]	
6175-49-1	2-dodecanone	C12H24O	[9, 247]			[182]			[110, 111, 420]	
593-08-8	2-tridecanone	C13H26O				[182]	[156]		[110, 111, 420]	
2345-27-9	2-tetradecanone	C14H28O				[182]			[111, 420]	
2345-28-0	2-pentadecanone	C15H30O				[182]			[111, 420]	
818-23-5	8-Pentadecanone	C15H30O		[253]						
18787-63-8	2-hexadecanone	C16H32O2				[182]			[111]	
79246-41-6	8-Octadecanone	C18H36O		[253]						

629-66-3	2-nonadecanone	C19H38O						[110]	
<i>Straight chain alkene ketones</i>									
78-94-4	3-buten-2-one / methyl vinyl ketone	C4H6O			[6, 106, 265, 286, 370, 406]	[409, 410]	[155]	[106]	[110]
625-33-2	3-penten-2-one / Methyl propenyl ketone	C5H8O	[9]	[194, 196, 255, 256]	[6, 377]				[110]
3102-33-8	3-Penten-2-one, (E)-	C5H8O			[277]			[106]	
1629-58-9	1-penten-3-one / ethyl vinyl ketone	C5H8O			[408]		[155, 163]		[110]
763-93-9	3-hexen-2-one	C6H10O			[369, 408]				
2497-21-4	4-hexen-3-one	C6H10O	[9]		[408]				
1629-60-3	1-hexene-3-one	C6H10O					[162]		
109-49-9	1-hexen-5-one	C6H10O			[408]				
24332-22-7	4-Hepten-2-one, (E)-	C7H12O			[388]				
1119-44-4	3-Hepten-2-one	C7H12O		[196]					
4312-99-6	1-octen-3-one	C8H14O		[208]			[153, 162-165]		110,
1669-44-9	3-octen-2-one	C8H14O	[9]	[196]			[163, 156]		
14129-48-7	4-octen-3-one	C8H14O					[156]		
27039-84-5	5-nonen-2-one	C9H16O			[383]				
32064-72-5	2-nonen-4-one	C9H16O				[178]			
14309-57-0	3-nonen-2-one	C9H16O							[118]
24415-26-7	1-nonen-3-one	C9H16O					[162]		
38284-27-4	3,5-octadien-2-one	C8H12O					[156]		
65767-22-8	(Z)-1,5-octadien-3-one	C8H12O					[162, 164, 165]		
63766-91-6	1,2,3-butatrien-1-one	C4H2O			[400]				
10575-41-4	4-hexyn-3-one	C6H8O			[408]				

<i>Aliphatic diones</i>									
431-03-8	2,3-butanedione / diacetyl	C4H6O2	[9, 216, 222, 223, 247, 248]	[194, 208, 255, 256, 258]	[6, 106, 263, 275, 277, 286, 311, 329, 406]	[162]	[106]	[110, 111, 115, 116]	[241]
600-14-6	2,3-pentanedione	C5H8O2	[9, 216, 247]	[256, 258]		[156]	[125]	[110, 111]	
4437-51-8	3,4-hexanedione	C6H10O2	[9]						
3848-24-6	2,3-hexanedione	C6H10O2	[9]		[377]		[125]	[110, 111]	
110-13-4	2,5-hexandione	C6H10O2			[408]	[176]			
96-04-8	2,3-heptanedione	C7H12O2	[9]					[110]	
585-25-1	2,3-octanedione	C8H14O2						[110]	
3214-41-3	2,5-octanedione	C8H14O2					[124, 131]		
14090-87-0	2,4-Octanedione	C8H14O2						[111]	
13757-90-9	6,7-dodecanedione	C12H22O2					[130]		
<i>Branched aliphatic ketones</i>									
563-80-4	3-methyl-2-butanone	C5H10O	[216, 248]	[194, 255, 256, 258]	[408]		[125]		[241]
814-78-8	3-methyl-3-buten-2-one	C5H8O		[194]	[408]			[110]	
565-62-8	3-methyl-2-penten-4-one	C6H10O			[408]				
25044-01-3	2-methyl-1-penten-3-one	C6H10O	[9]						
141-79-7	4-methyl-3-penten-2-one	C6H10O	[9]	[193, 196, 255, 256]	[408]	[410]		[113, 116]	
815-57-6	2,4-Pentanedione, 3-methyl	C6H10O2			[277]				
75-97-8	3,3-dimethyl-2-butanone	C6H12O		[194]					
63072-44-6	methyl pentanone ui	C6H12O					[155]		
565-69-5	2-methyl-3-pentanone	C6H12O	[9]	[194, 256, 258]				[111]	

565-61-7	3-methyl-2-pentanone	C6H12O	[9, 247, 216]	[193, 194, 196, 255, 256, 258]	[408]			[111]	
108-10-1	4-methyl-2-pentanone /methyl isobutyl ketone	C6H12O	[9, 216, 223]	[193, 196, 198, 250, 255, 256, 258]	[6, 261, 294, 322, 361, 374, 378]	[183, 191]	[123]	[110, 111, 113]	[241]
5891-25-8	2,2-dimethyl-pent-4-yn-3-one / 4,4-dimethyl-1-pentyn-3-one	C7H10O					[125]		
623-56-3	5-methyl-3-hexanone	C7H14O	[9]	[196, 194, 255-258]	[408]		[125]		
565-80-0	2,4-dimethyl-3-pentanone	C7H14O	[9]	[196]				[110, 111]	
564-04-5	2,2-dimethyl-3-pentanone	C7H14O		[194]					
2550-21-2	3-methylhexan-2-one	C7H14O		[257, 258]	[408]				
17042-16-9	4-methyl-3-hexanone	C7H14O	[247]	[193, 194]					
110-12-3	5-methyl-2-hexanone	C7H14O	[9, 247]	[254]				[110, 111]	[241]
105-42-0	4-methyl-2-hexanone	C7H14O	[216]		[408]			[113]	
7379-12-6	2-methyl-3-hexanone	C7H14O				[155]		[110, 111]	
1604-28-0	6-methyl-3,5-heptadien-2-one	C8H12O	[9, 222]			[178]			
110-93-0	6-methyl-5-hepten-2-one / 6-Methylhept-5-en-2-one	C8H14O	[9, 216, 222, 248]	[194, 196, 258]	[6, 275, 296, 370, 388, 406]	[176, 178, 183, 185, 187, 189, 190, 409, 410]	[124, 126]	[110, 111, 422]	
3002-23-1	6-methyl-2,4-heptanedione	C8H14O2	[9]					[111]	
6137-06-0	4-Methyl-2-heptanone	C8H16O		[196, 250]				[111]	[241]

624-42-0	6-methyl-3-heptanone	C8H16O	[194, 256]	[408]			
626-33-5	2-methyl-4-heptanone	C8H16O	[194, 196, 253]				
928-68-7	6-methyl-2-heptanone / 2-isooctanone	C8H16O	[223, 247, 248]	[408]	[156, 167]	[124]	[117]
18217-12-4	5-methyl-2-heptanone	C8H16O	[9]	[361]			[110]
1888-57-9	2,5-Dimethyl-3-hexanone	C8H16O					[111]
2371-19-9	3-methyl-2-heptanone	C8H16O	[257, 258]	[408]			
26118-38-7	3,3-dimethyl-2-hexanone	C8H16O	[258]				
29466-99-7	methyl heptanone ui	C8H16O			[155]		
541-85-5 / 20616-93-7	5-Methyl-3-heptanone	C8H16O					[111]
20633-03-8	3,4-Hexanedione, 2,2,5-trimethyl-	C9H16O2		[369, 377]	[409]		
na	7-Methyloctane-2,4-dione	C9H16O2					[111]
815-24-7	3-Pentanone, 2,2,4,4-tetramethyl-	C9H18O			[409]		
108-83-8	2,6-dimethyl-4-heptanone	C9H18O					[113]
na	5-Methyl-octanone	C9H18O					[111]
33933-82-3	5,9-Dimethyl-2-decanone	C12H24O					[111]
689-67-8	6,10-dimethyl-5,9-undecadien-2-one	C13H22O		[300]	[178, 185, 192, 409]		[112, 118]
3879-26-3 / 689-67-8	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	C13H22O					[111]
3796-70-1	geranylacetone / (E)-6,10-Dimethyl-5,9-undecadien-2-one	C13H22O	[253]		[176, 189, 190]	[156]	[118]





70286-20-3	dl-4-acetyl-1-methylcyclohexene	C9H14O	[196]	[408]				
na	1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)acetone	C12H20O	[253]					
1203-08-3	4-(2,6,6-trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	C13H18O	[194, 254]					
23726-93-4	beta-damascenone / 1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one	C13H18O	[193, 196, 202, 208, 250, 254]					
127-41-3	ionone (alpha) / 4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	C13H20O	[194]		[182]			[182, 420]
79-77-6	ionone (beta) / (3E)-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	C13H20O	[202, 193]	[300]	[182]	[162]		[420]
17283-81-7	4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone / dihydro-b-ionone	C13H22O	[254]					
79-68-5	gamma-irone / 4-(2,2,3-Trimethyl-6-methylenecyclohexyl)-3-buten-2-one	C14H22O			[182]			
127-43-5	1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-1-penten-3-one / b-methyl ionone	C14H22O	[254]					
79-69-6	(Z)-alpha-irone	C14H22O			[182]			[420]
ui	1-ethyl-3-methyl-b-ionone	unsure			[182]			
<i>Other aliphatic and aromatic ketones</i>								
88-29-9	7-acetyl-6-ethyl-1,1,4,4-tetramethyltetralin / musk 36A	C18H26O			[182]			

21145-77-7	2-acetyl-3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalene / Ethanone, 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthalenyl)-	C18H26O			[182, 409]		[182, 420]
3168-90-9	1-acetyl-2-methylcyclopentene / 1-(2-methyl-1-cyclopenten-1-yl)-ethanone	C8H12O					[110]
765-43-5	1-cyclopropylethanone	C5H8O		[194]	[364]		
<i>Hydroxy ketones</i>							
116-09-6	1-hydroxy-2-propanone / 1-Hydroxyacetone	C3H6O2	[9, 222]		[286, 298, 406, 408]		[114, 116]
513-86-0	3-hydroxy-2-butanone / acetoin	C4H8O2	[9, 223]		[263, 271, 276, 310, 311, 313, 322, 324, 329, 334, 367, 378, 408]	[190]	[111, 115, 116, 418] [241]
64502-89-2	1-Hydroxy-2-pentanone	C5H10O2		[254]			
5704-20-1	2-Hydroxy-3-pentanone / methylacetoin	C5H10O2					[111]
21856-89-3	6-hydroxyhexan-2-one	C6H12O2				[176]	
123-42-2	4-hydroxy-4-methyl-2-pentanone	C6H12O2					[125]
25368-54-1	8-Hydroxy-2-octanone	C8H16O2					[111]
582-24-1	2-hydroxy-1-phenylethanone	C8H8O2			[267]		
1075-06-5	2,2-dihydroxy-1-phenylethanone	C8H8O3	[222]				

3445-24-7	D-ribose	C5H8O5	[383]	
<i>Phenol ketones</i>				
99-93-4	1-(4-hydroxyphenyl)ethanone / piceol / 4'-hydroxyacetophenone	C8H8O2	[408]	[125]
708-23-6	5-Hydroxykynurenamine	C9H12N2O2	[45]	
720-00-3	5-Hydroxykynurenine	C10H12N2O4	[45]	
na	3-(Hydroxy-phenyl-methyl)-2,3-dimethyl-octan-4-one	C17H26O2	[277]	
14035-34-8	2,6-bis(1,1-dimethylethyl)-4-(1-oxopropyl) phenol	C17H26O2	[9]	[176]
76444-55-8	angoletin / 1-(2,4-dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenylpropan-1-one	C18H20O4	[383]	
3791-75-1	1-(2-hydroxy-4,6-dimethoxyphenyl)-3-(4-methoxyphenyl)propan-1-one / Flavokawin A	C18H20O5	[383]	
<i>Acid ketones</i>				
328-42-7	Oxalacetic acid	C4H4O5	[42]	
541-50-4	acetoacetic acid / 3-Oxobutanoic acid	C4H6O3	[383]	
328-50-7	2-Oxopentanedioic acid	C5H6O5	[42]	
na	Oxohexanoic acid u.i	C6H10O3	[43]	

3128-06-1	5-oxohexanoic acid / 5-Ketohexanoic acid	C6H10O3				[383]
na	4-(2-Aminophenyl)-2,4-dioxobutanoic acid / 4-(2-Aminophenyl)-2,4-dioxobutanoate	C10H9NO4				[45]
1022-31-7	N-Formylkynurenine	C11H12N2O 4				[45]
<i>Ketones with other functional groups</i>						
78-98-8	1,2-propanedione	C3H4O2				[408]
24653-75-6	mercaptoacetone	C3H6OS	[9, 248]			[408]
5878-19-3	2-Propanone, 1-methoxy / Methoxyacetone	C4H8O2				[241]
25016-16-4	1-(1H)-pyrazol-4-yl)-ethanone	C5H6N2O		[194]		
29926-41-8	1-(4,5-dihydro-2-thiazolyl)-ethanone	C5H7NOS	[9]			
141-97-9	acetoacetic acid, ethyl ester / ethyl acetotacetate / ethyl-3-oxobutanoate	C6H10O3				[122]
1696-20-4	1-morpholin-4-yl-ethanone	C6H11NO2				[408]
1192-62-7	2-acetylfuran / 1-(2-furanyl)-ethanone / furyl methyl ketone	C6H6O2	[9]	[193, 194, 196, 202, 250, 255, 256, 258]		[408] [155]
1072-83-9	Ethanone, 1-(1H-pyrrol-2-yl)- / 2-acetylpyrrole	C6H7NO				[341, 400]
85213-22-5	2-acetyl-1-pyrroline	C6H9NO		[208]		
89975-71-3	4-propoxy-2-butanone	C7H14O2				[408]
36687-99-7	3-ETHOXY-3-METHYL-2-BUTANONE	C7H14O2				[377]

33330-50-6	4-ethoxy-2-pentanone	C7H14O2	[256, 258]		
29006-00-6	2-Hexanone, 6-methoxy-	C7H14O2			[241]
123528-99-4	3,3-Dimethyl-4-methylamino-butan-2-one	C7H15NO			[241]
3194-15-8	1-(2-furyl)-1-propanone	C7H8O2		[408]	
1193-79-9	2-acetyl-5-methylfuran	C7H8O2	[9, 222]	[6, 275]	[110]
114-83-0	Acetohydroxamic Acid / Acetylphenylhydrazine	C8H10N2O			[241]
87773-62-4	3-Methyl-2-(2-oxopropyl)furan	C8H10O2			[241]
57545-63-8	4-sec-Butoxy-2-butanone	C8H16O2		[277]	
1074-12-0	phenylglyoxal	C8H6O2	[222]		
36357-38-7	5-acetyl-2-methylpyridine	C8H9NO	[9]		
613-89-8	2-aminoacetophenone	C8H9NO			[162]
24985-48-6	2-methoxy-2-octen-4-one	C9H16O2			[178]
2922-83-0	L-Kynurenine	C10H12N2O		[45]	
52450-38-1	Formyl-N-acetyl-5-methoxykynurenamine	C13H16N2O		[45]	
4620-54-6	1-phenyl-3-(1-piperidiny)-2-buten-1-one	C15H19NO			[178]
na	Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	C16H30O4	[253]		