

Table 3. List of sulphur-containing volatile organic compounds (VOCs) in human body.

CAS-number	Compound name	Formula	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva	Semen
13798-23-7	Hexathiane / Sulfur (S6) / Hexasulfur	S6			[61, 380]					
10544-50-0	Octasulfur	S8			[380]					
<i>Thiols</i>										
74-93-1	methanethiol / thiomethane / methyl mercaptan	CH4S	[9, 222, 223, 248]	[193, 194, 196, 202, 250, 258]	[6, 264, 268, 275, 325, 370, 378, 385, 389, 394]	[178]			[117]	[241]
68-11-1	mercaptoacetic acid / thioglycolic acid	C2H4O2S							[117]	
75-08-1	thioethanol	C2H6S			[408]					
60-23-1	cysteamine	C2H7NS			[308]					
24653-75-6	mercaptoacetone	C3H6OS	[9, 248,]		[408]					
870-23-5	allyl mercaptan	C3H6S		[194]	[283, 327]				[110]	
107-03-9	1-propanethiol	C3H8S	[9]	[194]	[324]				[117]	
75-66-1	2-methyl-2-propanethiol	C4H10S		[258]						
513-44-0	2-methylthiopropene	C4H10S							[117]	
227456-33-9	2-methyl-3-sulfanylbutan-1-ol	C5H12OS				[414]				
548740-99-4	3-sulfanylpentan-1-ol	C5H12OS				[414]				
616-31-9	3-pentanethiol	C5H12S2		[258]						
28588-74-1	2-methylmercaptofuran	C5H6OS		[193, 202]						
51755-83-0	2-sulfanylhexan-1-ol	C6H14OS				[414]				
149-30-4	2-mercaptobenzothiazole	C7H6NS2			[47]					
307964-23-4	3-methyl-3-sulfanylhexan-1-ol	C7H16OS				[414]				

7341-17-5	2-ethyl-1-hexanethiol	C8H18S	[248]						
3489-28-9	nonane-1,9-dithiol	C9H20S2			[383]				
33281-91-3	8-Mercapto-p-menthan-3one	C10H18OS			[29]				
112-55-0	1-thiododecane	C12H26S				[178]			
10059-13-9	2-Undecanethiol, 2-methyl-	C12H26S			[274]				
	<i>Sulfides, sulfanyl</i>								
7783-06-4	hydrogen sulfide	H2S	[9]	[252]	[134, 273, 278, 284, 293, 301, 307, 309, 316, 325, 330, 345, 347, 363, 378, 381, 394]			[134]	
75-15-0	carbon disulfide	CS2	[9, 222, 223, 247]	[258]	[6, 57, 264, 273, 278, 284, 301, 303, 307, 309, 330, 341, 345, 361, 380, 381, 387, 404, 406]	[178]	[155]	[127]	[113]

75-18-3	dimethylsulfide / thiopropane / DMS	C2H6S	[9, 216, 222, 223, 248]		[6, 57, 106, 264, 268, 273, 275, 278, 284, 286, 301, 307, 309, 316, 322, 325, 330, 338, 341, 345, 357, 363, 371, 378, 381, 385, 389, 394, 404, 406, 407]	[178, 410]	[106, 417]	[117]	[241]
624-92-0	dimethyldisulfide / methyldisulfide	C2H6S2	[9, 216, 222, 223, 247, 248,]	[193, 194, 196, 197, 198, 254, 202, 250, 255-258]	[61, 307, 309, 327, 351, 378, 380, 394]	[155]	[125]	[110, 111, 117, 418]	[241]
3658-80-8	dimethyltrisulfide	C2H6S3	[9, 216, 222, 223, 247, 248]	[193, 194, 196, 202, 208, 250, 253, 254, 257, 258]	[394]		[125]	[111, 117, 418]	[241]
5756-24-1	dimethyltetrasulfide	C2H6S4		[258]				[111]	
7330-31-6	Dimethyl pentasulfide	C2H6S5						[111]	
624-89-5	ethylmethylsulfide	C3H8S		[196, 258]	[6, 106]		[106]		
1618-26-4	2,4-dithiapentane	C3H8S2	[216]				[125]		
42474-44-2	methyl(methylthio)methyl disulfide	C3H8S3	[9]						
42848-06-6	1-(methylthio)-1-propene, (1E)-	C4H8S	[9]		[6, 265, 275, 322]			[110]	
52195-40-1	1-(methylthio)-1-propene, (Z)-	C4H8S			[6, 57]			[110]	

10152-76-8	allyl methylsulfide / 3-(methylthio)-1-propene /methylthiopropene	C4H8S		[194, 254]	[6, 57, 106, 283, 322, 325, 326, 327, 338, 363, 371, 407]	[410]	[168]	[106]	[110]
10152-77-9	methylthiopropene	C4H8S							117,
2179-58-0	allyl methyldisulfide / Disulfde methyl-2-propenyl	C4H8S2		[193, 196, 257, 258]	[283, 327]				
352-93-2	Diethylsulfide	C4H10S				[189]			
3877-15-4	1-(methylthio)-propane / methylpropylsulfide / 1-methyl thiopropane / methyl n-propyl sulfide	C4H10S	[9]		[6, 57, 106, 265, 322, 326, 363, 367, 378, 392]			[106]	[110]
22551-26-4	3-(methylthio)-1,2-propanediol	C4H10O2S				[178]			
505-10-2	3-(methylthio)-1-propanol	C4H10OS	[9]						
2179-60-4	methylpropyldisulfide	C4H10S2	[9, 216, 222]	[193, 194, 248]				[125]	
3268-49-3	3-(methylthio)-propanal / methional	C4H8OS	[9]	[197, 208]				[162, 164]	
59121-24-3	4-methylthiobutane nitrile	C5H9NS		[258]					
5454-45-5	3-(ethylthio)propanal	C5H10OS			[408]				
628-29-5	1-methylthiobutane	C5H12S2				[178]			
4396-19-4	1,1'-(methylene-bis(thio))bis ethane	C5H12S2		[258]					
20600-63-9	Acetic acid, (2-propenylthio)- ((Allylthio) acetic acid)	C5H8O2S							[241]
592-88-1	Diallyl sulphide	C6H10S		[254]					
2179-57-9	diallyl disulfide	C6H10S2		[194]	[283]				
117013-33-9	3-(ethylsulfanyl)butan-1-ol	C6H14OS			[383]				

629-19-6	dipropyldisulfide	C6H14S2	[9]				
33672-51-4	Isopropyl propyl disulphide	C6H14S2		[338]			
20651-30-3	5-methyl-2-methylthio-4(1H)-pyrimidinone	C6H8N2OS				[178]	
13678-59-6	2-methyl-5-(methylthio)furan	C6H8OS		[194, 202, 250]			
44657-76-3	2-methyl-2-[(1-methylethyl)thio]-propane	C7H16S		[193, 258]			
766-92-7	benzyl methyl sulphide	C8H10S					[125]
29549-68-6	o-2-(butenylthio)phenol	C10H12OS				[178]	
<i>Sulfoxide, sulfone</i>							
7446-09-5	sulfur dioxide	O2S		[260, 343, 368, 369, 408]		[155]	
463-58-1	carbonyl sulfide	COS		[6, 275, 322]		[155]	
67-71-0	dimethylsulfone	C2H6O2S		[196, 256, 258]	[176, 179, 180]		[111, 116]
67-68-5	dimethylsulfoxide	C2H6OS	[9]	[258]	[322, 408]		[141]
16215-14-8	Allyl methyl sulfone	C4H8O2S				[168]	
126-33-0	Thiophene, tetrahydro-, 1,1-dioxide	C4H8O2S		[29]			
n.a.	Allyl methyl sulfoxide	C4H8OS				[168]	
872-93-5	3-Methyl sulfolane	C5H10O2S		[254]			
43115-41-9	Phenol, 2-amino-5-(methylsulfonyl)	C7H9NO3S					[241]
3185-99-7	1-methyl-4-methylsulfonylbenzene	C8H10O2S					[125]
16823-61-3	Di(n-hexyl)sulfone	C12H26O2S		[369]			
<i>Sulfonic acid esters, sulfate esters</i>							
7664-93-9	sulfate / Sulfuric acid	H2O4S		[355]			

na	Sulfurous acid, cyclohexylmethyl hexyl ester	C13H26O3S		[304]		
na	Sulfurous acid, 2-ethylhexyl isohexyl ester	C14H30O3S		[369]	[409]	
959067-41-5	Sulfurous acid, 2-ethylhexyl hexyl ester	C14H30O3S		[277]		
152216-76-7	4,4'-Diisothiocyanatostilbene-2,2'-disulfonic acid	C16H10N2O6S4		[369]		[241]
77-78-1	dimethylsulfuric acid ester	C2H6O4S	[9]			
n/a	laureth sulfosuccinate	C(16+2n)H(28+4n)O(7+n)S 2Metal counterions		[355]		
<i>Thioesters</i>						
507-09-5	thioacetic acid	C2H4OS		[258]		
1534-08-3	ethanethioic acid, (S)-methyl ester	C3H6OS	[9]	[408]		[111, 117] [241]
5925-75-7	propanethioc acid, S-methyl ester / S-methyl propanethioate	C4H8OS	[9, 216]	[255]		
2432-51-1	butanethioic acid, (S)-methyl ester / 1-(methylsulfanyl)butan-1-one	C5H10OS	[9]	[383]		
23747-45-7	3-methylbutanethioc acid, S-methyl ester / methyl 3-methylbutanethioate	C6H12OS	[9, 216, 248]			
42075-43-4	S-Methyl pentanethioate	C6H12OS				[111]
5925-74-6	benzeneethanethioic acid, (S)-methyl ester	C9H10OS	[9]			
<i>Thione</i>						
758-16-7	dimethylthioformamide	C3H7NS		[408]		
2832-99-7	N-Thio-valero-morpholine	C9H17NOS				[241]

Heterocyclics (for those heterocyclics including Nitrogen see Nitrogen table 2c)*Thiirane [C2S]*

1072-43-1	methylthiirane / propylenesulfide	C3H6S	[193, 194, 256, 258]	[6, 106, 383, 403-408]
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Thietane [C3S]

22438-40-0	3-methylthietane	C4H8S		[178]
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Thiophene, thiolane [C4S]

110-02-1	thiophene	C4H4S	[256, 258]	[106, 380, 408]	[106]
1003-10-7	dihydro-2-(3H)-thiophenone / Thiolan-2-one	C4H6OS	[9]	[256, 258]	[111]
126-33-0	Thiophene, tetrahydro-, 1,1-dioxide	C4H8O2S		[29]	
872-93-5	3-Methyl sulfolane	C5H10O2S	[254]		
498-62-4	3-Thiophenecarboxaldehyde / 3-formylthiophene	C5H4OS		[341]	
16839-97-7	2-methoxythiophene	C5H6OS	[194, 250]		
7210-64-2	5-methyl-2(5H)-thiophenone	C5H6OS		[178]	
554-14-3	2-methylthiophene	C5H6S		[6]	
616-44-4	3-methylthiophene	C5H6S	[9, 222]	[6, 61, 106, 380]	[106]
5780-36-9	Thiophene 2-methylthio	C5H6S2	[196]		
31053-55-1	2-methoxy-5-methylthiophene	C6H8OS		[178]	
638-00-6	2,4-dimethylthiophene	C6H8S	[194, 258]		
632-15-5	3,4-dimethylthiophene	C6H8S	[194, 254]		
872-55-9	2-ethylthiophen	C6H8S		[408]	
4861-58-9	2-pentylthiophene	C9H14S			[113]
50-59-9	Cephaloridine	C19H17N3O4S2			[241]

<i>Thiane [C5S]</i>				
505-23-7	1,3-Dithio cyclohexane / 1,3-dithiane	C4H8S2	[254]	
<i>Dithiane [C4S2]</i>				
45411-69-6	1,3-dithiacyclohexene / 5,6-Dihydro-4H-1,3-dithiin-1-ium	C4H8S2	[193]	
<i>Oxathole [C3OS]</i>				
92572-53-7	4-Allyl-2-t-butyl-4-methyl-1,3-oxathiolan-5-one	C11H18O2S		[241]
<i>Oxadithiane [C3OS2]</i>				
53897-57-7	2,4,6-triethyl-1,3,5-oxadithiane	C9H18OS2	[383]	
