

Table 5b. Table showing the branched chain alkanes reported in the literature that have been detected in the healthy human body

CAS-number	Compound name	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva
75-28-5	2-methylpropane			Br				
78-78-4	2-methylbutane			Br				
75-83-2	2,2-dimethylbutane			Br				
79-29-8	2,3-dimethylbutane			Br				
464-06-2	2,2,3-trimethylbutane	F						
594-82-1	2,2,3,3-tetramethylbutane			Br				
107-83-5	2-methylpentane	F		Br			Bl	Sa
96-14-0	3-methylpentane	F		Br			Bl	Sa
590-35-2	2,2-dimethylpentane			Br				
565-59-3	2,3-dimethylpentane			Br				
108-08-7	2,4-dimethylpentane			Br				
562-49-2	3,3-dimethylpentane			Br				
540-84-1	2,2,4-trimethylpentane			Br			Bl	
560-21-4	2,3,3-trimethylpentane			Br				
564-02-3	2,2,3-trimethylpentane			Br				
565-75-3	2,3,4-trimethylpentane			Br				
617-78-7	3-ethylpentane			Br				
609-26-7	2-methyl-3-ethylpentane			Br				
589-34-4	3-methylhexane			Br				
591-76-4	2-methylhexane			Br				
590-73-8	2,2-dimethylhexane			Br				
584-94-1	2,3-dimethylhexane			Br				
589-43-5	2,4-dimethylhexane			Br	Sk			
592-13-2	2,5-dimethylhexane			Br				
563-16-6	3,3-dimethylhexane			Br				
1069-53-0	2,3,5-trimethylhexane			Br				
16747-26-5	2,2,4-trimethylhexane			Br				
3522-94-9	2,2,5-trimethylhexane			Br				
921-47-1	2,3,4-trimethylhexane			Br				
16747-30-1	2,4,4-trimethylhexane			Br				
619-99-8	3-ethylhexane			Br				
592-27-8	2-methylheptane			Br				Sa
589-81-1	3-methylheptane	F		Br				Sa
589-53-7	4-methylheptane			Br				
1071-26-7	2,2-dimethylheptane			Br				
3074-71-3	2,3-dimethylheptane			Br				
2213-23-2	2,4-dimethylheptane	F	U	Br				
2216-30-0	2,5-dimethylheptane			Br				
1072-05-5	2,6-dimethylheptane			Br				
926-82-9	3,5-dimethylheptane			Br				
2613-61-8	2,4,6-trimethylheptane			Br				
52896-95-4	2,3,4-trimethylheptane			Br				
7154-80-5	3,3,5-trimethylheptane							Sa
14676-29-0	2-methyl-3-ethylheptane			Br				
3221-61-2	2-methyloctane			Br				

CAS-number	Compound name	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva
2216-33-3	3-methyloctane			Br				
2216-34-4	4-methyloctane	F		Br				
15869-89-3	2,5-dimethyloctane			Br				
2051-30-1	2,6-dimethyloctane			Br				
1072-16-8	2,7-dimethyloctane			Br				
15869-93-9	3,5-dimethyloctane			Br				
15869-94-0	3,6-dimethyloctane			Br				
62016-14-2	2,5,6-trimethyloctane			Br				
62016-28-8	2,2,6-trimethyloctane			Br				
62016-33-5	2,3,6-trimethyloctane			Br				
62016-37-9	2,4,6-trimethyloctane			Br				
62183-79-3	2,2,4,4-tetramethyloctane			Br				
52670-34-5	2,3,6,7-tetramethyloctane	F		Br				
15869-86-0	4-ethyloctane			Br				
5881-17-4	3-ethyloctane			Br				
62016-18-6	5-ethyl-2-methyloctane			Br				
62016-19-7	6-ethyl-2-methyloctane	F		Br				
62183-55-5	3-ethyl-2,7-dimethyloctane			Br				
871-83-0	2-methylnonane	F		Br				
5911-04-6	3-methylnonane			Br				
17301-94-9	4-methylnonane			Br				
15869-85-9	5-methylnonane			Br				
17302-27-1	2,5-dimethylnonane			Br				
17302-28-2	2,6-dimethylnonane			Br				
17302-23-7	4,5-dimethylnonane			Br				
13151-34-3	2-ethylnonane			Br				
6975-98-0	2-methyldecane			Br				
2847-72-5	4-methyldecane			Br				
13151-35-4	5-methyldecane			Br				
17312-44-6	2,3-dimethyldecane			Br				
2801-84-5	2,4-dimethyldecane			Br				
13150-81-7	2,6-dimethyldecane			Br				
17312-45-7	3,4-dimethyldecane			Br				
17312-53-7	3,6-dimethyldecane			Br				
17312-54-8	3,7-dimethyldecane			Br				
17312-55-9	3,8-dimethyldecane			Br				
1636-43-7	5,6-dimethyldecane			Br				
62108-25-2	2,6,7-trimethyldecane			Br				
62108-26-3	2,6,8-trimethyldecane			Br				
62108-27-4	2,4,6-trimethyldecane	F		Br				
1636-44-8	4-ethyldecane			Br				
7045-71-8	2-methylundecane			Br				
1002-43-3	3-methylundecane			Br				
2980-69-0	4-methylundecane	F		Br				
1632-70-8	5-methylundecane			Br				
17301-32-5	4,7-dimethylundecane	F		Br				
17312-83-3	5,7-dimethylundecane			Br				
31295-56-4	2,6,11-trimethyldodecane	F						

CAS-number	Compound name	Faeces	Urine	Breath	Skin	Milk	Blood	Saliva
ui	propyldodecane				Sk			
2801-87-8	4-methylpentadecane				Sk			Sa
158274-95-4	methyl heptadecane				Sk			
6561-44-0	3-methyloctadecane				Sk			Sa
6418-45-7	3-methylnonadecane				Sk			

NOTES ui unidentified isomer