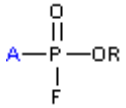
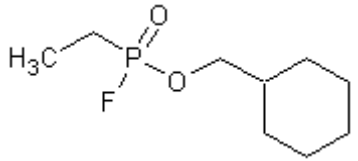
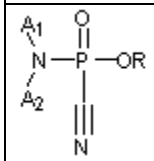
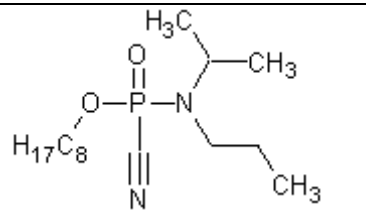
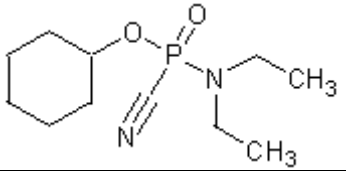
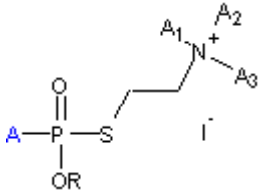
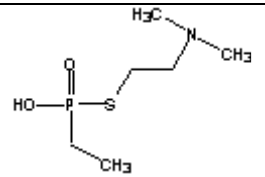
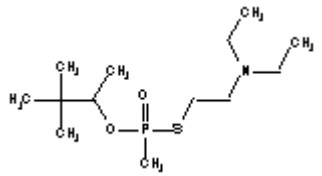
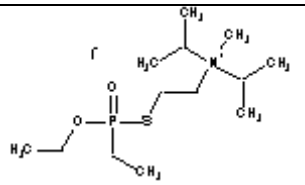
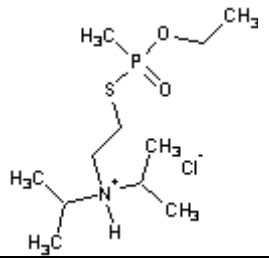
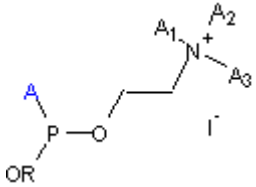
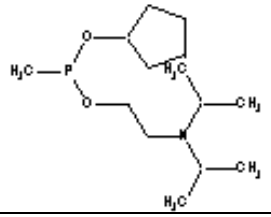
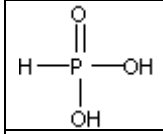
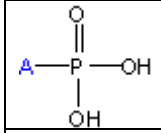
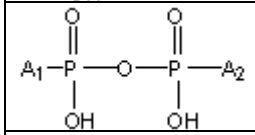
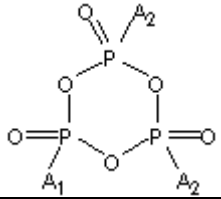
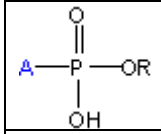
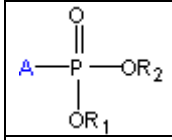
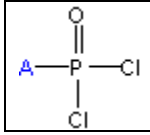
GUIDELINES FOR ASSIGNEMENT OF THE CHEMICAL KEY CODE TO THE SCHEDULED CHEMICALS IN THE HANDBOOK ON CHEMICALS DATABASE.

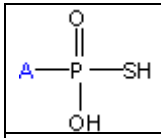
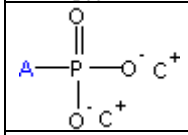
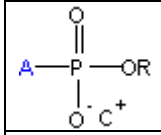
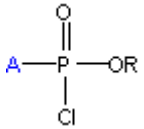
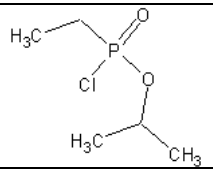
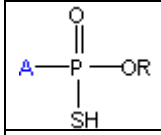
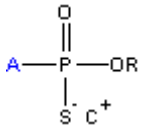
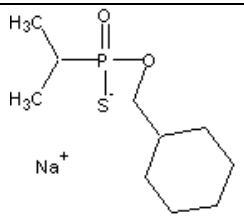
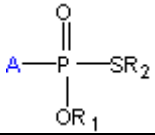
The default Key Code is the CAS Registry Number. If the chemical doesn't have a CAS Registry Number, the Key is generated in accordance with the following general indications:

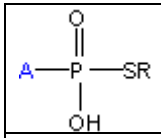
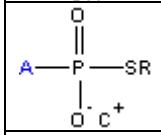
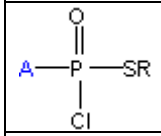
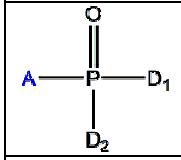
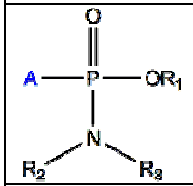
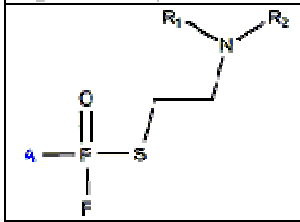
- The parent structure is indicated with the schedule number: 1A1, 1A2, etc... For the 2B4 compounds there are five large families from the compounds declared: 2B41(phosphonic acid derivatives), 2B42(phosphinic acid derivatives), 2B43(phosphonous acid derivatives), 2B44(phosphinous acid derivatives) and 2B45(phosphonothioic acid derivatives).
- There are two main types of substituents:
  - an alkyl radical (attached to P or N, or O in the 2B6 family) which is always limited to Me, Et, n-Pr and i-Pr. This substituent will appear in the code as M, E, P or I and is indicated in the general structure with an A.
  - a radical which is always attached to O or S. This substituent will be indicated in the code as a CAS number in brackets and is the CAS number of the original alcohol ROH (see list of alcohols and CAS RN in the appendix) It is indicated in the general structure as (R).
- Other substituents like Cl, SH, $O^-(C^+)$ or $S^-(C^+)$, X (always attached to the P) are indicated as such.
- A, A_1, A_2, A_3 = Me, Et, n-Pr or i-Pr and is indicated with the letters M, E. P and I. A_n are written in alphabetical order.
- (R) or (R_n) means CAS registry number of the parent alcohol. In the 1A3 and 1B10 families R can also be hydrogen, in which case it is indicated with H.
- S(R_n) means CAS registry number of the parent alcohol from which the thiol could be derivatised.
- N(R1) means CAS registry number of the parent alcohol of alkyl R1 from which an amine could be derivatised.
- I- indicates the anion (e.g. Cl, I).
- C+ indicates the cation. When it is a metallic cation the chemical symbol of the element is indicated (i.e. Na, K). When the cation is a compound, the CAS number of the original compound is indicated (e.g. 7664-41-7 for NH_3 or 101-83-7 for Dicyclohexylamine).
- When the molecule is optically active, the sign (+) or (-) is added at the end of the code after a hyphen.
- Hydrogen isotopes are added to the code at the end of the relevant part of the Key with indication of the number of isotopes (e.g. –T3, –D7). Carbon isotopes are also added to the end of the relevant part of the Key with an indication of the position of the isotopes where known (e.g. [1,2-14C]
- When the CAS number of the original alcohol is not available, the chemical code is indicated by a 4 digit number ID.(i.e. ID1351)

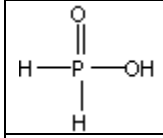
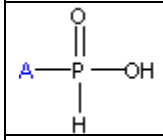
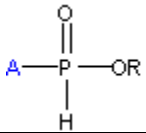
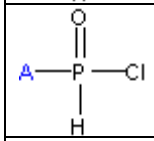
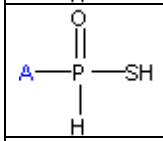
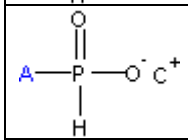
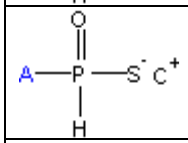
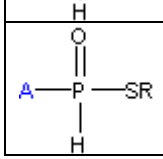
Chemical structure	Name	Code	Chemical structure	Code
	O-Alkyl alkylphosphonofluoridates	(R)-A**1A1**		(100-49-2)-E**1A1**
	O-Alkyl N,N-dialkylphosphoramidocyanidates	(R)-1A2-A_1A_2	 	(111-87-5)-1A2-IP (108-93-0)-1A2-EE
	O-Alkyl S-2-dialkylaminoethyl alkyl phosphonothiolates and corresponding alkylated or protonated salts	(R)-A1A3-$A_1A_2A_3(I^-)$	 	H-E1A3-MM (464-07-3)-M1A3-EE (64-17-5)-E1A3-IIM(I)

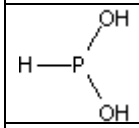
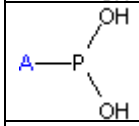
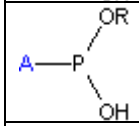
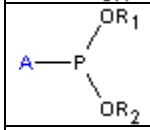
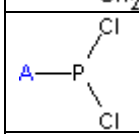
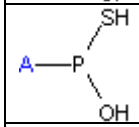
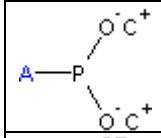
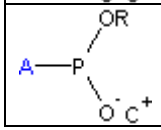
			 	(64-17-5)-M1A3-IIH(Cl)
	O-Alkyl O-2-dialkylaminoethyl alkyl phosphonites and corresponding alkylated or protonated salts	(R)-A1B10-$A_1A_2A_3(I^-)$		(96-41-3)-M1B10-II

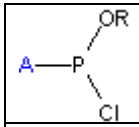
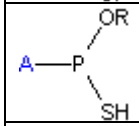
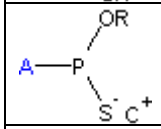
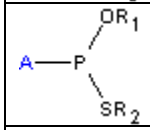
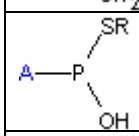
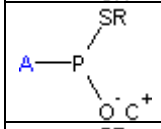
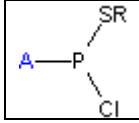
Chemical structure	Name	Code	Chemical structure	Code
	Phosphonic acid (Not a schedule compound)	2B41		
	Alkylphosphonic acid	A2B41		
	$Alkyl_1alkyl_2$phosphonic anhydride	$A_1A_2$2B41		
	$Alkyl_1alkyl_2alkyl_3$phosphonic tricyclic anhidride	$A_1A_2A_3$2B41		
	Monoester	(R)-A2B41		
	Diester	(R_1)-A2B41-(R_2)		
	Dichloride	Cl-A2B41-Cl		

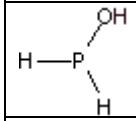
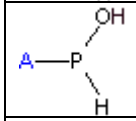
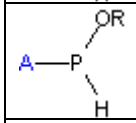
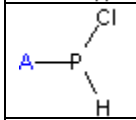
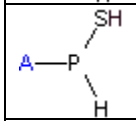
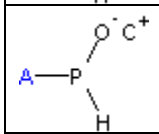
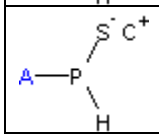
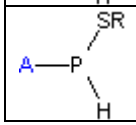
	Monothiol	SH-A2B41		
	Salt	A2B41-O(C^+)-O(C^+)		
	Monoester salt	(R)-A2B41-O(C^+)		
	Monoester chloride	(R)-A2B41-Cl		(67-63-0)-E2B41-Cl
	Monoester thiol	(R)-A2B41-SH		
	Monoester thiol salt	(R)-A2B41-S(C^+)		(100-49-2)-I2B41-S(Na)
	Monoester thiolate	(R_1)-A2B41-S(R_2)		

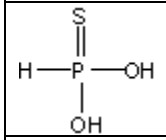
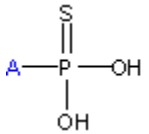
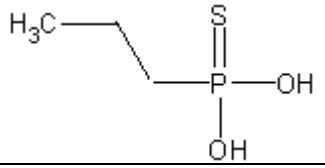
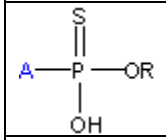
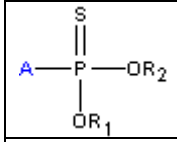
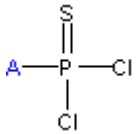
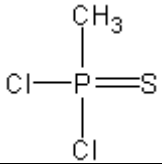
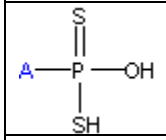
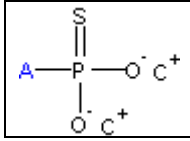
	Thiolate	S(R)-A2B41		
	Thiolate salt	S(R)-A2B41-O(C^+)		
	Thiolate chloride	S(R)-A2B41-Cl		
	General structure	(D1)-A2B41-(D2)		
	Alkyl N,N-Dialkyl alkylphosphonoamidate	(R1)-A2B41-N(R2)(R3)		(108-93-0)-M2B41-N(65-56-1)(107-21-1)
	S-2-Dialkylaminoethyl alkylphosphonothionofluoridate	S[N(R1)(R2)]-A2B41-F		S[N(64-17-5)(64-17-5)]-M2B41-F

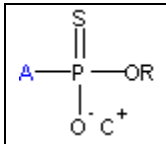
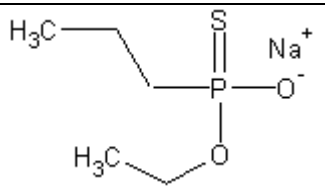
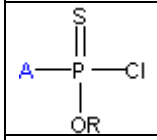
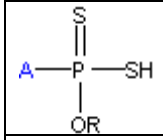
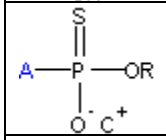
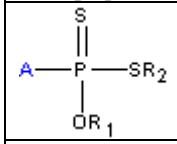
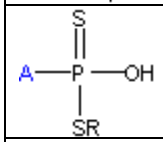
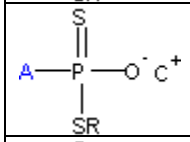
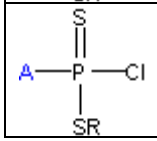
Chemical structure	Name	Code	Chemical structure	Code
	Phosphinic acid (Not a schedule compound)	2B42		
	Alkylphosphinic acid	A2B42		
	Ester	(R)-A2B42		
	Chloride	Cl-A2B42		
	Thiol	SH-A2B42		
	Salt	A2B42-O(C^+)		
	Thiol salt	A2B42-S(C^+)		
	Thiolate	S(R)-A2B42		

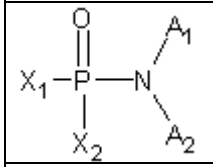
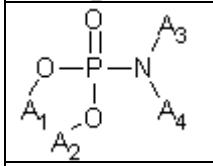
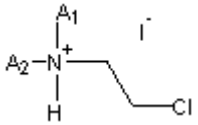
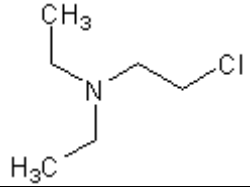
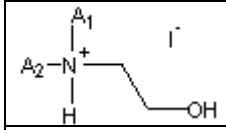
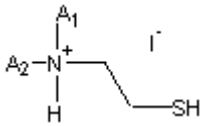
Chemical structure	Name	Code	Chemical structure	Code
	<u>Phosphonous acid</u> (Not a schedule compound)	<u>2B43</u>		
	Alkylphosphonous acid	A2B43		
	‘Monoester’	(R)-A2B43		
	‘Diester’	(R_1)-A2B43-(R_2)		
	Dichloride	Cl-A2B43-Cl		
	Monothiol	SH-A2B43		
	Salt	A2B43-O(C^+)		
	‘Monoester’ salt	(R)-A2B43-O(C^+)		

	‘Monoester’ chloride	(R)-A2B43-Cl		
	‘Monoester’ thiol	(R)-A2B43-SH		
	‘Monoester’ thiol salt	(R)-A2B43-S(C^+)		
	‘Monoester’ thiolate	(R_1)-A2B43-S(R_2)		
	Thiolate	S(R)-A2B43		
	Thiolate salt	S(R)-A2B43-O(C^+)		
	Thiolate chloride	S(R)-A2B43-Cl		

Chemical structure	Name	Code	Chemical structure	Code
	Phosphinous acid (Not a schedule compound)	2B44		
	Alkylphosphinous acid	A2B44		
	‘Ester’	(R)-A2B44		
	Chloride	Cl-A2B44		
	Thiol	SH-A2B44		
	Salt	A2B44-O(C^+)		
	Thiol salt	A2B44-S(C^+)		
	Thiolate	S(R)-A2B44		

Chemical structure	Name	Code	Chemical structure	Code
	Phosphonothioic acid	2B45		
	Alkylphosphonothioic acid	A2B45		P2B45
	Monoester	(R)-A2B45		
	Diester	(R_1)-A2B45-(R_2)		
	Dichloride	Cl-A2B45-Cl		Cl-M2B45-Cl
	Monothiol	SH-A2B45		
	Salt	A2B45-O(C^+)		

	Monoester salt	(R)-A2B45-O(C^+)		(64-17-5)-P2B45-O(Na)
	Monoester chloride	(R)-A2B45-Cl		
	Monoester thiol	(R)-A2B45-SH		
	Monoester thiol salt	(R)-A2B45-S(C^+)		
	Monoester thiolate	(R_1)-A2B45-S(R_2)		
	Thiolate	S(R)-A2B45		
	Thiolate salt	S(R)-A2B45-O(C^+)		
	Thiolate chloride	S(R)-A2B45-Cl		

Chemical structure	Name	Code	Chemical structure	Code
	N,N-Dialkyl phosphoramidic dihalides	X_1-X_2-2B5-A_1A_2		
	Dialkyl N,N-dialkylphosphoramidates	A_1-A_2-2B6-A_3A_4		
	N,N-Dialkyl aminoethyl-2-chlorides and corresponding protonated salts	2B10-$A_1A_2(I^-)$		2B10-EE
	N,N-Dialkyl aminoethane-2-ols and corresponding protonated salts	2B11-$A_1A_2(I^-)$		
	N,N-Dialkyl aminoethane-2-thiols and corresponding protonated salts	2B12-$A_1A_2(I^-)$		

APPENDIX: LIST OF ALCOHOLS AND CAS RN

Alcohol	Radical	CAS
2,3-Dimethyl-2-butanol	1,1,2-trimethylpropyl	594-60-5
2,6-Dimethyl-2-heptanol	1,1,5-trimethylhexyl	13254-34-7
3-Ethyl-2,2-dimethyl-3-pentanol	1,1-diethyl-2,2-dimethylpropyl	66793-96-2
3-Ethyl-3-pentanol	1,1-diethylpropyl	597-49-9
2-Methyl-2-pentanol	1,1-dimethylbutyl	590-36-3
1,1-Dimethylpentanol	1,1-Dimethylpentyl	28929-86-4
2-Methyl-2-hexanol	1,1-dimethylpentyl	625-23-0
2-Methyl-2-butanol	1,1-dimethylpropyl	75-85-4
3,3-Dimethyl-2-pentanol	1,2,2-trimethylbutyl	19781-24-9
3,3-dimethyl-2-butanol	1,2,2-trimethylpropyl	464-07-3
3-Methyl-2-pentanol	1,2-dimethylbutyl	565-60-6
3-Methyl-2-butanol	1,2-dimethylpropyl	598-75-4
4,4-Dimethyl-2-pentanol	1,3,3-trimethylbutyl	6144-93-0
4-Methyl-2-pentanol	1,3-dimethylbutyl	108-11-2
5-Methyl-2-Hexanol	1,4-dimethylpentyl	627-59-8
3,7-Dimethyloctan-3-ol	1,5-dimethyl-1-ethylhexyl	57706-88-4
6-Methyl-2-heptanol	1,5-dimethylhexyl	4730-22-7
5-Nonanol	1-butylpentyl	623-93-8
1-Cyclohexylethanol	1-cyclohexylethyl	1193-81-3
1-Cyclopropylethanol	1-cyclopropylethyl	765-42-4
3-Methyl-3-heptanol	1-ethyl-1-methylpentyl	5582-82-1
3-Methyl-3-pentanol	1-Ethyl-1-methylpropyl	77-74-7
2,2-Dimethyl-3-pentanol	1-ethyl-2,2-dimethylpropyl	3970-62-5
4-Methyl-3-hexanol	1-ethyl-2-methylbutyl	615-29-2
4-Methyl-3-heptanol	1-ethyl-2-methylpentyl	14979-39-6
2-Methyl-3-pentanol	1-ethyl-2-methylpropyl	565-67-3
3-Hexanol	1-ethylbutyl	623-37-0
3-Nonanol	1-ethylheptyl	624-51-1
3-Octanol	1-ethylhexyl	20296-29-1
3-Heptanol	1-ethylpentyl	589-82-2
3-Pentanol	1-ethylpropyl	584-02-1
2,6-Dimethyl-4-heptanol	1-isobutyl-3-methylbutyl	108-82-7
2,4-Dimethyl-3-pentanol	1-isopropyl-2-methylpropyl	600-36-2
2-Methyl-3-hexanol	1-isopropylbutyl	617-29-8
2-Pentanol	1-methylbutyl	6032-29-7
1-Methylcyclohexanol	1-methylcyclohexyl	590-67-0
2-Octanol	1-methylheptyl	123-96-6
2-Heptanol	1-methylhexyl	543-49-7
2-Decanol	1-methylnonyl	1120-06-5
2-Nonanol	1-methyloctyl	628-99-9
2-Hexanol	1-methylpentyl	626-93-7
2-Butanol	1-methylpropyl	78-92-2
4-Heptanol	1-propylbutyl	589-55-9
4-Decanol	1-propylheptyl	2051-31-2
4-Octanol	1-propylpentyl	589-62-8
2-(Diisopropylamino)ethanol	2-(diisopropylamino)ethyl	96-80-0
2,2-Dimethylcyclohexanol	2,2-dimethylcyclohexyl	69542-91-2
2,2-Dimethylhexanol	2,2-dimethylhexyl	2370-13-0
2,2-Dimethylpropanol	2,2-dimethylpropyl	75-84-3

2,3-Dimethylbutanol	2,3-dimethylbutyl	19550-30-2
2,3-Dimethylcyclohexanol	2,3-dimethylcyclohexyl	1502-24-5
2,3-Dimethylpentanol	2,3-dimethylpentyl	10143-23-4
2,4,4-Trimethylpentanol	2,4,4-trimethylpentyl	16325-63-6
2,4-Dimethylcyclohexanol	2,4-dimethylcyclohexyl	1193-46-0
2,5-Dimethylcyclohexanol	2,5-dimethylcyclohexyl	3809-32-3
2,6-Dimethylcyclohexanol	2,6-dimethylcyclohexyl	5337-72-4
2-Cyclohexylethanol	2-cyclohexylethyl	4442-79-9
2-Cyclopentylethanol	2-cyclopentylethyl	766-00-7
2-Ethylbutanol	2-ethylbutyl	97-95-0
2-Ethylcyclohexanol	2-ethylcyclohexyl	3760-20-1
2-Ethylhexanol	2-ethylhexyl	104-76-7
Ethane-1,2-diol	2-hydroxyethanol	107-21-1
2-Isopropyl-3-methylbutanol	2-isopropyl-3-methylbutyl	18593-92-5
2-Isopropyl-5-methylcyclohexanol	2-isopropyl-5-methylcyclohexyl	89-78-1
2-Methylbutanol	2-methylbutyl	137-32-6
2-Methylcyclohexanol	2-methylcyclohexyl	583-59-5
2-Methylcyclopentanol	2-methylcyclopentyl	24070-77-7
2-Methylhexanol	2-methylhexyl	624-22-6
2-Methylpentanol	2-methylpentyl	105-30-6
2-Methylpropanol	2-methylpropyl	78-83-1
2-Propylpentanol	2-propylpentyl	58175-57-8
2-tert-Butylcyclohexanol	2-tert-butylcyclohexyl	13491-79-7
3,3,5,5-Tetramethylcyclohexanol	3,3,5,5-tetramethylcyclohexyl	2650-40-4
3,3-Dimethylbutanol	3,3-dimethylbutyl	624-95-3
3,3-Dimethylcyclohexanol	3,3-dimethylcyclohexyl	767-12-4
3,4,4-Trimethylhexanol	3,4,4-trimethylhexyl	66793-73-5
3,5,5-Trimethylhexanol	3,5,5-trimethylhexyl	3452-97-9
3,5,5-Trimethylhexanol	3,5,5-trimethylhexyl	3452-97-9
3,5-Dimethylcyclohexanol	3,5-dimethylcyclohexyl	5441-52-1
3,7-Dimethyloctanol	3,7-dimethyloctyl	106-21-8
3-Cyclohexylpropanol	3-cyclohexylpropyl	1124-63-6
3-Cyclopentylpropanol	3-cyclopentylpropyl	767-05-5
3-Methylbutanol	3-methylbutyl	123-51-3
3-Methylcyclohexanol	3-methylcyclohexyl	591-23-1
3-Methylcyclopentanol	3-methylcyclopentyl	18729-48-1
3-Methylpentanol	3-methylpentyl	589-35-5
4-Cyclohexylbutanol	4-cyclohexylbutyl	4441-57-0
4-Ethylcyclohexanol	4-ethylcyclohexyl	4534-74-1
4-Methylcyclohexanol	4-methylcyclohexyl	589-91-3
4-Methylpentanol	4-methylpentyl	626-89-1
4-tert-Butylcyclohexanol	4-tert-butylcyclohexyl	98-52-2
5-Isopropyl-2-methylcyclohexanol	5-isopropyl-2-methylcyclohexyl	60320-28-7
Phenylmethanol	Bencyl	100-51-6
1-Butanol	butyl	71-36-3
Cyclobutanol	cyclobutyl	2919-23-5
Cycloheptanol	cycloheptyl	502-41-0
Cyclohexanol	cyclohexyl	108-93-0
Cyclohexanol-d13	cyclohexyl-d13	66522-78-9
Cyclohexylmethanol	cyclohexylmethyl	100-49-2
Cyclooctanol	cyclooctyl	696-71-9
Cyclopentanol	cyclopentyl	96-41-3

Cyclopentylmethanol	cyclopentylmethyl	3637-61-4
Cyclopropylmethanol	cyclopropylmethyl	2516-33-8
Decanol	decyl	112-30-1
Ethanol	ethyl	64-17-5
Ethanol-d6	ethyl-d6	1516-08-1
1-Heptanol	heptyl	111-70-6
1-Hexanol	hexyl	111-27-3
2-Methylpropanol	isobutyl	78-83-1
2-Propanol	isopropyl	67-63-0
Isopropanol-d8	isopropyl-d8	22739-76-0
Methanol	methyl	67-56-1
	N-ethylbenzenaminium	103-69-5
1-Nonanol	nonyl	143-08-8
Octanol	octyl	111-87-5
1-Pentanol	pentyl	71-41-0
Pinacolyl alcohol	pinacolyl	464-07-3
1-Propanol	propyl	71-23-8
2-Methyl-2-propanol	tert-butyl	75-65-0