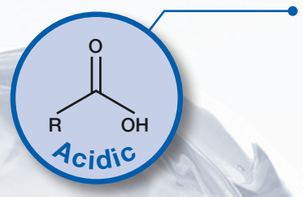
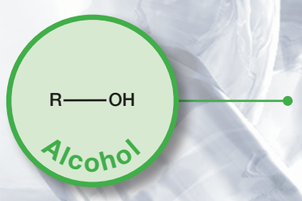
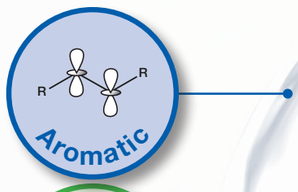
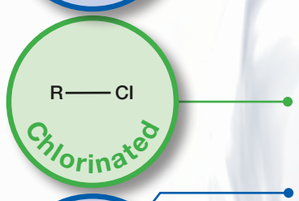
NMR Proton Shifts for Residual Solvent Impurities

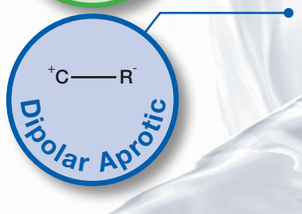
Solvent Type

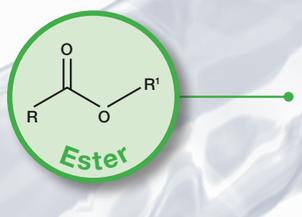


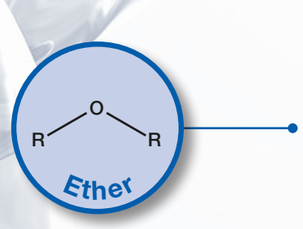


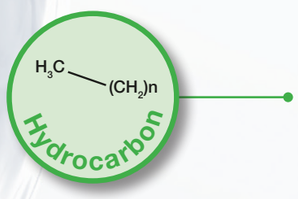


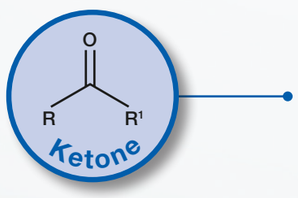


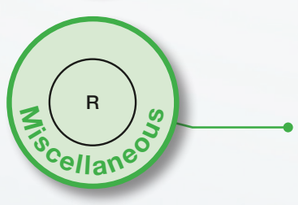












Solvent	Synonyms	Mol Wt	BP °C	Linear Formula	H-Signal	Multi	$CDCl_3$	D_2O	CD_3OD	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	C_6D_6
Acetic Acid	Ethanoic acid	60.05	118	CH_3COOH	CH_3	s	2.13	2.08	1.99	1.95	1.96	1.96	1.55
Formic Acid	Methanoic Acid	46.02	101	HCOOH	H	s	8.02	8.22	8.08	8.18	8.11	8.03	–
1-Butanol	*n*-Butanol / 1-Hydroxybutane / *n*-Butyl alcohol	74.12	117.6	$CH_3(CH_2)_3OH$	CH_3	t	0.94	0.91	0.93	0.86	0.90	0.91	–
					CH_2 (3)	m	1.39	1.35	1.38	1.30	1.31-1.41	1.29-1.39	–
					CH_2 (2)	m	1.56	1.53	1.51	1.39	1.44-1.52	1.42-1.49	–
					CH_2 (1)	m	3.65	3.61	3.54	3.38	3.49-3.56	3.45-3.51	–
2-Butanol	*sec*-Butanol / 2-Butyl alcohol / 2-Hydroxybutane	74.12	99	$CH_3CH(OH)CH_2CH_3$	CH_3 (4)	t	0.93	0.84	0.91	0.83	0.89	0.88	–
					CH_3 (1)	d	1.19	1.11	1.13	1.02	1.09	1.08	–
					CH_2	m	1.48	1.42	1.44	1.32	1.33-1.47	1.33-1.42	–
					CH	m	3.73	3.71	3.63	3.49	3.56-3.66	3.54-3.62	–
tert-Butanol	*t*-Butyl alcohol / 2-Methyl-2-propanol	74.12	83	$(CH_3)_3COH$	CH_3	s	1.28	1.24	1.40	1.11	1.18	1.16	1.05
Ethanol	Ethyl alcohol	46.06	78	C_2H_6O	CH_3	t	1.25	1.17	1.19	1.06	1.12	1.12	0.96
					CH_2	q	3.72	3.65	3.60	3.44	3.57	3.54	3.34
Ethylene Glycol	Ethane-1,2-diol / 1,2-Dihydroxyethane	62.06	196-198	$HOCH_2CH_2OH$	CH	s	3.76	3.65	3.59	3.34	3.28	3.51	3.41
1-Hexanol	*n*-Hexanol / Hexyl alcohol / Caproic alcohol	102.18	156-157	$CH_3(CH_2)_5OH$	CH_3	t	0.86-0.93	0.88	0.87-0.94	0.86	0.88	0.89	–
					CH_2 (3-5)	m	1.24-1.44	1.24-1.39	1.26-1.40	1.19-1.32	1.24-1.39	1.22-1.38	–
					CH_2 (2)	m	1.52-1.61	1.50-1.59	1.48-1.57	1.36-1.44	1.45-1.55	1.43-1.51	–
					CH_2 (1)	m	3.64	3.69	3.53	3.35-3.40	3.37	3.44-3.50	–
iso-Amyl alcohol	3-Methyl-1-butanol / *iso*-Pentyl alcohol	88.15	130	$(CH_3)_2CHCH_2CH_2OH$	CH_3	d	0.92	0.90	0.91	0.85	0.89	0.89	–
					CH_2CH	q	1.47	1.44	1.42	1.31	1.39	1.37	–
					CH	m	1.66-1.78	1.61-1.71	1.64-1.77	1.65	1.72	1.67	–
					CH_2OH	m	3.68	3.64	3.58	3.41	3.53-3.59	3.51	–
iso-Butanol	*iso*-Butyl alcohol / 2-Methyl-1-propanol	74.12	108	$(CH_3)_2CHCH_2OH$	CH_3	d	0.92	0.88	0.90	0.82	0.87	0.86	–
					CH	m	1.77	1.75	1.70	1.60	1.68	1.66	–
					CH_2	m	3.41	3.38	3.30	3.15	3.26-3.34	3.25	–
Methanol	Methyl alcohol	32.04	64.7	CH_3OH	CH_3	s	3.49	3.34	3.34	3.16	3.31	3.28	3.07
Pentanol	*n*-Amyl alcohol / Pentyl alcohol	88.15	137-139	$CH_3(CH_2)_4OH$	CH_3	t	0.91	0.88	0.92	0.86	0.89	0.90	–
					CH_2 (3-4)	m	1.31	1.31	1.34	1.27	1.27-1.37	1.25-1.38	–
					CH_2 (2)	m	1.58	1.55	1.53	1.41	1.45-1.55	1.43-1.52	–
					CH_2 (1)	t	3.64	3.60	3.53	3.37	3.37	2.46	–
1-Propanol	*n*-Propanol / Propyl alcohol	60.10	97	$CH_3CH_2CH_2OH$	CH_3	t	0.93	0.90	0.92	0.87	0.89	0.88	–
					CH_2 (2)	m	1.60	1.55	1.54	1.45	1.44-1.55	1.43-1.52	–
					CH_2 (1)	t	3.60	3.56	3.49	3.38	3.44-3.51	3.40-3.47	–
2-Propanol	IPA / Isopropanol / *iso*-Propyl alcohol	60.10	82	$(CH_3)_2CHOH$	CH_3	d	1.20	1.18	1.14	1.04	1.10	1.09	0.95
					CH	m	4.03	4.02	3.92	3.78	3.90	3.67	3.87
Anisole	Methoxybenzene / Methyl phenyl ether	108.14	154	$C_6H_5OCH_3$	CH_3	s	3.76	3.85	3.77	3.76	3.78	3.77	–
					CH (*o/p*)	m	6.93	7.06	6.90	6.93	6.88-6.95	6.89-6.98	–
					CH (*m*)	m	7.29	7.41	7.25	7.29	7.24-7.31	7.27-7.34	–
Benzene		78.11	80.09	C_6H_6		s	7.37	7.44	7.33	7.37	7.36	7.37	7.15
Pyridine		79.10	115-116	C_5H_5N	CH (2)	m	8.62	8.52	8.53	8.58	8.58	8.57	8.53
					CH (3)	m	7.29	7.45	7.44	7.39	7.35	7.33	6.66
					CH (4)	m	7.68	7.87	7.85	7.79	7.76	7.73	6.98
Toluene	Methylbenzene	92.14	111	$C_6H_5CH_3$	CH_3	s	2.36	–	2.32	2.30	2.32	2.33	2.11
					CH (*o/p*)	m	7.17	–	7.16	7.18	7.10-7.20	7.10-7.30	7.02
					CH (*m*)	m	7.25	–	7.16	7.25	7.10-7.20	7.10-7.30	7.13
p-Xylene	1,4-Dimethylbenzene / *p*-Xylol	106.17	138	$C_6H_4(CH_3)_2$	CH_3	s	2.30	2.30	2.26	2.24	2.26	2.27	–
					CH	s	7.06	7.18	7.02	7.05	–	–	–
Chloroform	Trichloromethane / Formyl trichloride	119.38	61	$CHCl_3$	CH	s	7.26	–	7.88	8.32	8.02	7.58	6.15
1,2-Dichloroethane	EDC / Ethylene dichloride / Glycol dichloride	98.96	81-85	$ClCH_2CH_2Cl$	CH_2	s	3.73	–	3.78	3.90	3.87	3.81	2.90
Dichloromethane	DCM / Methylene dichloride	84.93	39-40	CH_2Cl_2	CH_2	s	5.30	–	5.48	5.76	5.63	5.44	4.27
Acetonitrile	AcCN / Methyl cyanide / Cyanomethane	41.04	81-82	CH_3CN	CH_3	s	2.10	2.06	2.03	2.07	2.05	1.96	1.55
Dimethylformamide	DMF / Formyldimethylamine	73.09	153	$HCON(CH_3)_2$	CH	s	8.02	7.91	7.98	7.95	7.96	7.92	7.63
					CH_3	s	2.96	3.00	2.99	2.89	2.94	2.89	2.36
					CH_3	s	2.88	2.86	2.85	2.73	2.78	2.77	1.86
Dimethyl sulfoxide	DMSO / Methyl sulfoxide / (Methylsulfinyl)methane	78.13	189	$(CH_3)_2SO$	CH_3	s	2.62	2.71	2.65	2.54	2.52	2.50	1.68
n-Butyl acetate	1-Butyl acetate	116.16	126-127	$CH_3CO_2(CH_2)_3CH_3$	CH_3CH_2	t	0.94	0.91	0.94	0.89	0.92	0.92	–
					CH_2	m	1.38	1.37	1.39	1.32	1.32-1.43	1.31-1.42	–
					CH_2	m	1.61	1.63	1.61	1.54	1.54-1.62	1.54-1.63	–
					CH_3CO	s	2.04	2.09	2.01	1.99	1.97	1.97	–
					CH_2CO	t	4.07	4.11	4.06	3.99	4.02	4.02	–
Ethyl acetate	EtOAc / Ethyl ethanoate / Acetoxyethane	88.11	75-78	$CH_3CO_2C_2H_5$	CH_3CH_2	t	1.26	1.24	1.24	1.18	1.20	1.20	0.92
					CH_3CO	s	2.05	2.07	2.01	1.99	1.97	1.97	1.65
					CH_2	q	4.12	4.14	4.09	4.03	4.05	4.06	3.89
Ethyl formate	Ethyl methanoate / Formic acid ethyl ester	74.08	54	$HCO_2C_2H_5$	CH_3	t	1.29	1.29	1.27	1.24	–	–	–
					CH_2	q	4.22	4.28	4.20	4.17	–	–	–
					CH	s	8.04	8.16	8.06	8.23	–	–	–
iso-Propyl acetate	iPrOAc / 1-Methyl ethyl acetate / 2-Propyl acetate	102.13	88.8	$CH_3CO_2CH(CH_3)_2$	$(CH_3)_2CH$	d	1.23	1.25	1.22	1.17	1.19	1.19	–
					CH_3CO	s	2.02	2.07	1.99	1.96	1.94	1.94	–
					CH	m	4.99	4.98	4.95	4.86	4.91	4.91	–
Methyl acetate	Methyl ethanoate / Methyl acetic ester	74.08	57.4	$CH_3CO_2CH_3$	CH_3CO	s	2.05	2.09	2.02	1.92	1.98	1.99	–
					OCH_3	s	3.67	3.68	3.64	3.61	3.59	3.60	–
n-Propyl acetate	Acetic acid propyl ester / Propyl ethanoate	102.13	102	$CH_3CO_2CH_2CH_2CH_3$	CH_3CH_2	t	0.94	0.92	0.94	0.88	0.92	0.92	–
					CH_2CH_3	m	1.65	1.65	1.64	1.57	1.61	1.61	–
					CH_3CO	s	2.05	2.09	2.02	2.00	1.98	1.98	–
					CH_2CO	t	4.02	4.06	4.01	3.95	3.97	3.97	–
tert-Butyl methyl ether	MTBE / 2-Methyl-2-methoxy propane	88.15	54-56	$(CH_3)_3COCH_3$	CCH_3	s	1.19	1.22	1.15	1.11	1.19	1.14	1.07
					OCH_3	s	3.22	3.24	3.20	3.08	3.13	3.13	3.04
Diethyl ether	Ether / Ethoxyethane	74.12	34.6	$(CH_3CH_2)_2O$	CH_3	t	1.20	1.17	1.17	1.09	1.11	1.12	1.11
					CH_2	q	3.48	3.56	3.49	3.38	3.41	3.42	3.26
1,2-Dimethoxyethane	DME / Dimethylglycol	90.12	84-86	$CH_3OCH_2CH_2OCH_3$	CH_3	s	3.40	3.37	3.35	3.24	3.28	3.28	3.24
					CH_2	s	3.55	3.60	3.52	3.43	3.46	3.45	3.33
1,4-Dioxane	Diethylene ether / Diethylene dioxide	88.11	101	$C_4H_8O_2$	CH_2	s	3.71	3.75	3.66	3.57	3.59	3.60	3.35
Tetrahydrofuran	THF / Oxolane / Diethylene oxide	72.11	66	C_4H_8O	CH_2	m	1.85	1.88	1.87	1.76	1.79	1.80	1.40
					CH_2O	m	3.76	3.74	3.71	3.60	3.63	3.64	3.57
Cyclohexane		84.16	81	C_6H_{12}	CH_2	s	1.43	–	1.45	1.40	1.43	1.44	1.40
n-Heptane	Heptane / Dipropyl methane	100.21	98	$CH_3(CH_2)_5CH_3$	CH_3	t	0.89	–	0.90	0.86	0.88	0.89	–
					CH_2	m	1.28	–	1.31	1.26	1.21-1.35	1.21-1.35	–
n-Hexane		86.18	69	$CH_3(CH_2)_4CH_3$	CH_3	t	0.88	–	0.90	0.86	0.88	0.89	0.89
					CH_2	m	1.26	–	1.29	1.25	1.28	1.28	1.24
Methylcyclohexane	MCH	98.19	101	$CH_3CH(CH_2)_5$	CH_2CH (ax)	m	0.82-0.93	–	0.82-0.94	0.80-0.90	0.87-0.93	0.88-0.94	–
					CH_3	d	0.86	–	0.87	0.84	0.84	0.86	–
					CH_2 (4) (ax)	m	1.06-1.17	–	1.09-1.20	1.04-1.14	1.07-1.17	1.08-1.18	–
					CH_2 (3) (ax)	m	1.17-1.28	–	1.26	1.14-1.25	1.24	1.25	–
					CH	m	1.33	–	1.31-1.39	1.32	1.34	1.30-1.39	–
n-Pentane		72.15	36	$CH_3(CH_2)_3CH_3$	CH_3	t	0.88	–	0.90	0.86	0.88	0.89	0.87
					CH_2	m	1.27	–	1.29	1.27	1.27	1.29	1.23
Acetone	2-Propanone / Dimethylketone	58.08	56	CH_3COCH_3	CH_3	s	2.17	2.22	2.15	2.09	2.09	2.08	1.55
2-Hexanone	MBK / Methyl butyl ketone / Propyl acetone	100.16	127	$CH_3(CH_2)_3COCH_3$	CH_3	t	0.91	0.88	0.91	0.85	–	–	–
					CH_2	m	1.32	1.30	1.32	1.24	–	–	–
					CH_2	m	1.56	1.53	1.53	1.43	–	–	–
					CH_2CO	t	2.42	2.56	2.47	2.41	–	–	–
					CH_3CO	s	2.13	2.21	2.12	2.07	–	–	–
Isobutyl methyl ketone	MIBK / 4-Methylpentan-2-one / Isopropylacetone	100.16	117.4	$(CH_3)_2CHCH_2COCH_3$	$(CH_3)_2CH$	d	0.92	0.90	0.85	0.85	0.88	0.88	–
					CH	m	2.13	2.08	2.00	2.00	2.02-2.11	2.02-2.08	–
					CH_3CO	s	2.12	2.21	2.05	2.05	2.06	2.05	–
					CH_2	d	2.30	2.43	2.28	2.28	2.31	2.29	–
Methyl ethyl ketone	MEK / Ethyl methyl ketone / 2-Butanone	72.11	80	$C_2H_5COCH_3$	CH_3CH_2	t	1.06	1.26	1.01	0.91	0.96	0.96	0.85
					CH_3CO	s	2.14	2.19	2.12	2.07	2.07	2.06	1.58
					CH_2CH_3	q	2.46	3.18	2.50	2.43	2.45	2.43	1.81
Triethylamine	TEA / Diethylaminoethane	101.19	90	$(C_2H_5)_3N$	CH_3	t	1.03	0.99	1.05	0.93	0.96	0.96	0.96
					CH_2	q	2.53	2.57	2.58	2.43	2.45	2.45	2.40
Formamide	Methanamide / Formic amide	45.04	210	$HCONH_2$	CH	s	8.22	8.06	8.04	7.97	–	–	–
Grease	Long chain, linear aliphatic hydrocarbons				CH_3	m	0.86	–	0.88	–	0.87	0.86	0.92
					CH_2	br s	1.26	–	1.29	–	1.29	1.27	1.36
Silicone Grease	Poly(dimethylsiloxane)				CH_3	s	0.07	–	0.10	–	0.13	0.08	0.29
Water		18.02	100	H_2O	H_2O	s	1.56	–	4.87	3.33	2.84	2.13	–

References - *Green Chem*., 2016, **18,** 3867-3878. *Magn. Reson. Chem*., 2005, **43**, 497-509. *J. Org. Chem*., 1997, **62**(1), 7512 -7515.

Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

GHS**01**
Explosive

- Self-reactives (severe)
- Organic peroxides

GHS**02**
Flammable

- Pyrophorics
- Self-reactives
- Self-heating
- In contact with water liberates flammable gases
- Organic peroxides

GHS**03**
Oxidizing

- May cause fire or explosion
- Strong oxidizer
- May intensify fire

GHS**04**
Compressed Gas

- Gas under pressure

GHS**05**
Corrosive

- Skin corrosives/burns
- Eye damage
- Corrosives to metals

GHS**06**
Toxic

- Acute toxicity (fatal or toxic)

GHS**07**
Harmful or Irritant

- Irritation (skin or eyes)
- Skin sensitizer
- Acute toxicity (harmful)
- Specific target organ toxicity – single exposure (drowsiness or dizziness or respiratory irritation)
- Hazardous to the ozone layer

GHS**08**
Health Hazard

- Carcinogen
- Respiratory sensitizer
- Reproductive toxicity
- Specific target organ toxicity – single or repeated exposure
- Germ cell mutagenicity
- Aspiration toxicity

GHS**09**
Hazardous to the Environment

- Hazardous to the aquatic environment (acute or long term)

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