

Propanal, 2-methyl-

Other names:	2-METHYLPROPANAL
	2-Methyl-1-propanal
	2-Methylpropionaldehyde
	2-methylpropanal (isobutanal)
	ISOBUTANAL
	ISOPROPYLFORMALDEHYDE
	Isobutaldehyde
	Isobutylaldehyde
	Isobutyral
	Isobutyraldehyd
	Isobutyraldehyde
	Isobutyric aldehyde
	Isobutyryl aldehyde
	Isopropylaldehyde
	Methyl propanal
	NCI-C60968
	NSC 6739
	Propionaldehyde, 2-methyl-
	UN 2045
	Valine aldehyde
	iso-C3H7CHO
	«alpha»-Methylpropionaldehyde
	Â«alphaÂ»-Methylpropionaldehyde
Inchi:	InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3
InchiKey:	AMIMRNSIRUDHCM-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	CC(C)C=O
Mol. weight [g/mol]:	72.11
CAS:	78-84-2

Physical Properties

Property code	Value	Unit	Source
af	0.3500		KDB
affp	797.30	kJ/mol	NIST Webbook
basg	765.50	kJ/mol	NIST Webbook
chl	-2469.40 ± 0.70	kJ/mol	NIST Webbook

chl	-2467.20 ± 0.75	kJ/mol	NIST Webbook
gf	-121.40	kJ/mol	KDB
hf	-215.70 ± 1.30	kJ/mol	NIST Webbook
hf	-218.00	kJ/mol	NIST Webbook
hf	-215.80 ± 1.50	kJ/mol	NIST Webbook
hf	-215.90	kJ/mol	KDB
hf	-216.40	kJ/mol	NIST Webbook
hfl	-247.30 ± 0.92	kJ/mol	NIST Webbook
hfl	-247.90 ± 0.70	kJ/mol	NIST Webbook
hfl	-247.20 ± 1.30	kJ/mol	NIST Webbook
hfl	-250.20 ± 0.75	kJ/mol	NIST Webbook
hfus	4.88	kJ/mol	Joback Method
hvap	32.30	kJ/mol	NIST Webbook
hvap	31.50 ± 1.30	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	32.00	kJ/mol	NIST Webbook
hvap	32.80	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	32.20	kJ/mol	NIST Webbook
ie	9.74 ± 0.03	eV	NIST Webbook
ie	9.69 ± 0.01	eV	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.71 ± 0.01	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.71 ± 0.02	eV	NIST Webbook
log10ws	-0.54		Crippen Method
logp	0.841		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	4150.00	kPa	KDB
rinpol	557.00		NIST Webbook
rinpol	532.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	554.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	595.00		NIST Webbook

rinpol	555.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	555.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	551.00	NIST Webbook
rinpol	548.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	535.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	552.00	NIST Webbook
rinpol	533.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	591.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	551.00	NIST Webbook
rinpol	535.00	NIST Webbook
rinpol	552.00	NIST Webbook
rinpol	544.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	537.00	NIST Webbook
rinpol	531.00	NIST Webbook
rinpol	546.00	NIST Webbook
rinpol	552.00	NIST Webbook
rinpol	561.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	551.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	553.00	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	536.00	NIST Webbook
rinpol	528.00	NIST Webbook
rinpol	567.00	NIST Webbook
rinpol	542.00	NIST Webbook
rinpol	541.00	NIST Webbook
rinpol	540.00	NIST Webbook

rinpol	543.00	NIST Webbook
rinpol	541.57	NIST Webbook
rinpol	540.94	NIST Webbook
rinpol	540.32	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	551.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	542.98	NIST Webbook
rinpol	582.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	531.00	NIST Webbook
rinpol	531.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	534.00	NIST Webbook
rinpol	538.00	NIST Webbook
rinpol	536.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	554.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	538.00	NIST Webbook
rinpol	541.00	NIST Webbook
rinpol	539.00	NIST Webbook
rinpol	537.00	NIST Webbook
rinpol	532.00	NIST Webbook
rinpol	536.00	NIST Webbook
rinpol	531.00	NIST Webbook
rinpol	530.00	NIST Webbook
rinpol	536.00	NIST Webbook
rinpol	547.00	NIST Webbook
rinpol	558.00	NIST Webbook
rinpol	538.00	NIST Webbook
rinpol	556.00	NIST Webbook
rinpol	543.00	NIST Webbook
rinpol	566.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	540.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	550.00	NIST Webbook

rinpol	547.00	NIST Webbook
rinpol	552.00	NIST Webbook
rinpol	550.00	NIST Webbook
rinpol	558.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	819.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	807.00	NIST Webbook
ripol	823.00	NIST Webbook
ripol	813.00	NIST Webbook
ripol	842.00	NIST Webbook
ripol	801.00	NIST Webbook
ripol	842.70	NIST Webbook
ripol	817.00	NIST Webbook
ripol	824.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	825.00	NIST Webbook
ripol	830.00	NIST Webbook
ripol	834.00	NIST Webbook
ripol	821.00	NIST Webbook
ripol	812.00	NIST Webbook
ripol	830.00	NIST Webbook
ripol	808.00	NIST Webbook
ripol	819.00	NIST Webbook
ripol	819.00	NIST Webbook
ripol	800.00	NIST Webbook
ripol	818.00	NIST Webbook
ripol	820.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	813.00	NIST Webbook
ripol	817.00	NIST Webbook
ripol	807.00	NIST Webbook
ripol	822.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	827.00	NIST Webbook
ripol	834.00	NIST Webbook
ripol	821.00	NIST Webbook
ripol	819.00	NIST Webbook
ripol	814.00	NIST Webbook
ripol	833.00	NIST Webbook
ripol	850.00	NIST Webbook
ripol	821.00	NIST Webbook

ripol	819.00		NIST Webbook
ripol	821.00		NIST Webbook
ripol	821.00		NIST Webbook
ripol	834.00		NIST Webbook
ripol	802.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	830.00		NIST Webbook
ripol	812.00		NIST Webbook
ripol	812.00		NIST Webbook
ripol	814.00		NIST Webbook
ripol	807.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	810.00		NIST Webbook
ripol	789.00		NIST Webbook
ripol	830.00		NIST Webbook
ripol	823.00		NIST Webbook
ripol	855.00		NIST Webbook
ripol	770.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	812.00		NIST Webbook
ripol	813.00		NIST Webbook
ripol	770.00		NIST Webbook
ripol	828.00		NIST Webbook
ripol	813.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	838.60		NIST Webbook
ripol	836.80		NIST Webbook
ripol	830.40		NIST Webbook
ripol	842.70		NIST Webbook
ripol	812.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	831.00		NIST Webbook
tb	336.20	K	NIST Webbook
tb	337.00	K	KDB
tb	334.15 ± 3.00	K	NIST Webbook
tb	335.15 ± 2.00	K	NIST Webbook
tb	336.65 ± 2.00	K	NIST Webbook

tb	334.15 ± 2.00	K	NIST Webbook
tb	334.15 ± 2.00	K	NIST Webbook
tb	335.15 ± 3.00	K	NIST Webbook
tb	337.15 ± 2.00	K	NIST Webbook
tb	335.65 ± 2.00	K	NIST Webbook
tb	336.45 ± 1.00	K	NIST Webbook
tb	336.85 ± 1.00	K	NIST Webbook
tb	337.25 ± 1.00	K	NIST Webbook
tb	336.20 ± 2.00	K	NIST Webbook
tb	337.00 ± 3.00	K	NIST Webbook
tb	336.70 ± 0.60	K	NIST Webbook
tb	337.65 ± 2.00	K	NIST Webbook
tb	336.65 ± 1.00	K	NIST Webbook
tb	337.15 ± 1.00	K	NIST Webbook
tb	337.25 ± 1.00	K	NIST Webbook
tb	335.15 ± 0.50	K	NIST Webbook
tb	337.20 ± 2.00	K	NIST Webbook
tb	64.33 ± 0.10	K	NIST Webbook
tb	337.15 ± 2.00	K	NIST Webbook
tb	337.25	K	NIST Webbook
tb	381.15 ± 0.40	K	NIST Webbook
tb	342.02 ± 0.30	K	NIST Webbook
tb	337.70	K	NIST Webbook
tb	336.65 ± 2.00	K	NIST Webbook
tc	513.00	K	KDB
tf	207.30 ± 2.00	K	NIST Webbook
tf	208.20	K	KDB
tf	207.30 ± 0.40	K	NIST Webbook
tf	145.00 ± 3.00	K	NIST Webbook
tf	207.30 ± 2.00	K	NIST Webbook
tf	201.00 ± 0.50	K	NIST Webbook
tf	201.00 ± 0.50	K	NIST Webbook
vc	0.274	m3/kmol	KDB
zc	0.2665900		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.16	J/mol×K	486.81	Joback Method
cpg	126.02	J/mol×K	398.21	Joback Method
cpg	119.12	J/mol×K	368.67	Joback Method

cpg	111.96	J/mol×K	339.14	Joback Method
cpg	132.65	J/mol×K	427.74	Joback Method
cpg	151.04	J/mol×K	516.35	Joback Method
cpg	139.03	J/mol×K	457.28	Joback Method
dvisc	0.0054155	Pa×s	161.84	Joback Method
dvisc	0.0002795	Pa×s	339.14	Joback Method
dvisc	0.0003619	Pa×s	309.59	Joback Method
dvisc	0.0004948	Pa×s	280.04	Joback Method
dvisc	0.0007282	Pa×s	250.49	Joback Method
dvisc	0.0011886	Pa×s	220.94	Joback Method
dvisc	0.0022568	Pa×s	191.39	Joback Method
hvapt	31.80	kJ/mol	323.00	NIST Webbook
hvapt	31.40	kJ/mol	318.50	NIST Webbook
hvapt	33.40	kJ/mol	340.00	NIST Webbook
rhoI	789.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48847e+01
Coeff. B	-3.01099e+03
Coeff. C	-4.27150e+01
Temperature range (K), min.	248.99
Temperature range (K), max.	357.24

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.23749e+02
Coeff. B	-7.99301e+03
Coeff. C	-1.67410e+01
Coeff. D	1.78146e-05
Temperature range (K), min.	208.15
Temperature range (K), max.	508.46

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1235
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of Henry's Law Constants for Acetone, 2-Butanone, 2-Pentanone, and Isobutyraldehyde Using a Horizontal Flow Reactor:	https://www.doi.org/10.1021/je034137r
KDB Vapor Pressure Data:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1235
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78842&Units=SI
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://en.wikipedia.org/wiki/Joback_method
Solubility Measurement and Correlation of Carbon Monoxide (CO) in Butyraldehydes: n-Butyraldehyde and iso-Butyraldehyde:	https://www.cheric.org/files/research/kdb/mol/mol1235.mol
	https://www.doi.org/10.1021/acs.jced.6b00765

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

Latest version available from:

<https://www.cheméo.com/cid/69-912-3/Propanal-2-methyl.pdf>

Generated by Cheméo on 2025-12-23 06:14:25.908200465 +0000 UTC m=+6218663.438241134.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.