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	-2467.20 ± 0.75	kJ/mol	NIST Webbook

chl	-2469.40 ± 0.70	kJ/mol	NIST Webbook
gf	-121.40	kJ/mol	KDB
hf	-218.00	kJ/mol	NIST Webbook
hf	-215.90	kJ/mol	KDB
hf	-216.40	kJ/mol	NIST Webbook
hf	-215.70 ± 1.30	kJ/mol	NIST Webbook
hf	-215.80 ± 1.50	kJ/mol	NIST Webbook
hfl	-247.90 ± 0.70	kJ/mol	NIST Webbook
hfl	-247.30 ± 0.92	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	32.00	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	32.80	kJ/mol	NIST Webbook
hvap	32.20	kJ/mol	NIST Webbook
hvap	31.50 ± 1.30	kJ/mol	NIST Webbook
ie	9.82	eV	NIST Webbook
ie	9.74 ± 0.03	eV	NIST Webbook
ie	9.69 ± 0.01	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.71 ± 0.02	eV	NIST Webbook
ie	9.71 ± 0.01	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	550.00		NIST Webbook
rinpol	546.00		NIST Webbook
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ripol	830.40		NIST Webbook
ripol	842.70		NIST Webbook
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ripol	842.70		NIST Webbook
tb	336.20	K	NIST Webbook
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tb	337.15 ± 2.00	K	NIST Webbook
tb	64.33 ± 0.10	K	NIST Webbook
tb	337.20 ± 2.00	K	NIST Webbook

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tb	381.15 ± 0.40	K	NIST Webbook
tb	342.02 ± 0.30	K	NIST Webbook
tc	513.00	K	KDB
tf	207.30 ± 2.00	K	NIST Webbook
tf	145.00 ± 3.00	K	NIST Webbook
tf	207.30 ± 0.40	K	NIST Webbook
tf	201.00 ± 0.50	K	NIST Webbook
tf	208.20	K	KDB
tf	201.00 ± 0.50	K	NIST Webbook
tf	207.30 ± 2.00	K	NIST Webbook
vc	0.274	m3/kmol	KDB
zc	0.2665900		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.96	J/mol×K	339.14	Joback Method
cpg	119.12	J/mol×K	368.67	Joback Method
cpg	126.02	J/mol×K	398.21	Joback Method

cpg	132.65	J/mol×K	427.74	Joback Method
cpg	139.03	J/mol×K	457.28	Joback Method
cpg	145.16	J/mol×K	486.81	Joback Method
cpg	151.04	J/mol×K	516.35	Joback Method
dvisc	0.0011886	Pa×s	220.94	Joback Method
dvisc	0.0022568	Pa×s	191.39	Joback Method
dvisc	0.0054155	Pa×s	161.84	Joback Method
dvisc	0.0007282	Pa×s	250.49	Joback Method
dvisc	0.0004948	Pa×s	280.04	Joback Method
dvisc	0.0003619	Pa×s	309.59	Joback Method
dvisc	0.0002795	Pa×s	339.14	Joback Method
hvapt	31.40	kJ/mol	318.50	NIST Webbook
hvapt	31.80	kJ/mol	323.00	NIST Webbook
hvapt	33.40	kJ/mol	340.00	NIST Webbook
rhol	789.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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(Pvp) = 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78842&Units=SI
Measurement of Henry s Law Constants for Acetone, 2-Butanone, 2,3-Butanedione, and Isobutyraldehyde Using a Horizontal Flow Reactor:	https://www.doi.org/10.1021/je034137r
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1235.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1235
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Measurement and Correlation of Carbon Monoxide (CO) in Butyraldehydes: n-Butyraldehyde and iso-Butyraldehyde:	https://www.doi.org/10.1021/acs.jced.6b00765
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1235
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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