2-Propenal

Other names:	2-Propen-1-one
	2-Propenaldehyde
	Acraldehyde
	Acraldehydeacroleina
	Acrolein
	Acroleina
	Acroleine
	Acrylaldehyd
	Acrylaldehyde
	Acrylic Aldehyde
	Akrolein
	Akroleina
	Aldehyde acrylique
	Aldeide acrilica
	Allyl aldehyde
	Aqualin
	Aqualine
	CH2=CHCHO
	Crolean
	Ethylene aldehyde
	Magnacide
	Magnacide H
	NSC 8819
	Prop-2-En-1-al
	Propenal
	Propylene aldehyde
	Rcra waste number P003
	Slimicide
	UN 1092
Inchi:	InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2
InchiKey:	HGINCPLSRVDWNT-UHFFFAOYSA-N
Formula:	C3H4O
SMILES:	C=CC=O
Mol. weight [g/mol]:	56.06
CAS:	107-02-8

Physical Properties

Property code	Value	Unit	Source
af	0.3300		KDB
affp	797.00	kJ/mol	NIST Webbook
aigt	507.04	K	KDB
basg	765.10	kJ/mol	NIST Webbook
chl	-1632.00	kJ/mol	NIST Webbook
dm	2.90	debye	KDB
fll	2.80	% in Air	KDB
flu	31.00	% in Air	KDB
fpc	255.37	K	KDB
fpo	248.15	K	KDB
gf	-65.19	kJ/mol	KDB
hf	-70.92	kJ/mol	KDB
hfus	4.54	kJ/mol	Joback Method
hvap	28.32	kJ/mol	Joback Method
ie	10.14 ± 0.06	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.11 ± 0.01	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
ie	10.13	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	10.10 ± 0.01	eV	NIST Webbook
log10ws	0.57		Estimated Solubility Method
logp	0.371		Crippen Method
mcvol	50.400	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=2)		KDB
pc	5160.00	kPa	KDB
rinpol	463.00		NIST Webbook
rinpol	453.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	450.00		NIST Webbook
rinpol	459.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	470.00		NIST Webbook

rinpol	470.00		NIST Webbook
rinpol	446.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	464.00		NIST Webbook
rinpol	462.00		NIST Webbook
rinpol	463.00		NIST Webbook
ripol	876.10		NIST Webbook
ripol	867.00		NIST Webbook
ripol	869.40		NIST Webbook
ripol	871.80		NIST Webbook
ripol	828.00		NIST Webbook
ripol	851.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	838.00		NIST Webbook
ripol	876.10		NIST Webbook
ripol	864.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	828.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	852.00		NIST Webbook
tb	325.60 ± 0.60	K	NIST Webbook
tb	325.42 ± 0.02	K	NIST Webbook
tb	325.70 ± 0.50	K	NIST Webbook
tb	326.15	K	NIST Webbook
tb	370.05 ± 0.60	K	NIST Webbook
tb	326.00	K	KDB
tb	323.00 ± 2.00	K	NIST Webbook
tb	325.30 ± 0.40	K	NIST Webbook
tb	325.70	K	NIST Webbook
tc	506.00	K	KDB
tf	184.65 ± 1.00	K	NIST Webbook
tf	185.50 ± 0.40	K	NIST Webbook
tf	186.15	K	NIST Webbook
tf	186.00	K	KDB
vc	0.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	70.79	J/mol×K	313.38	Joback Method
cpg	75.32	J/mol×K	342.75	Joback Method
cpg	79.65	J/mol×K	372.12	Joback Method
cpg	83.80	J/mol×K	401.49	Joback Method
cpg	87.75	J/mol×K	430.86	Joback Method
cpg	91.53	J/mol×K	460.23	Joback Method
cpg	95.13	J/mol×K	489.60	Joback Method
dvisc	0.0006769	Pa×s	213.67	Joback Method
dvisc	0.0010567	Pa×s	188.74	Joback Method
dvisc	0.0018888	Pa×s	163.81	Joback Method
dvisc	0.0004759	Pa×s	238.59	Joback Method
dvisc	0.0003577	Pa×s	263.52	Joback Method
dvisc	0.0002824	Pa×s	288.45	Joback Method
dvisc	0.0002315	Pa×s	313.38	Joback Method
hvapt	32.30	kJ/mol	278.00	NIST Webbook
hvapt	33.50	kJ/mol	267.00	NIST Webbook
hvapt	30.90	kJ/mol	314.50	NIST Webbook
rhol	839.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45115e+01
Coeff. B	-2.99517e+03
Coeff. C	-2.72480e+01
Temperature range (K), min.	237.82
Temperature range (K), max.	352.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.74670e+01

Coeff. B	-6.25326e+03
Coeff. C	-1.12525e+01
Coeff. D	1.36307e-05
Temperature range (K), min.	185.45
Temperature range (K), max.	506.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1251
Measurement of activity coefficient at infinite dilution for some bio-oil components in water and mass transfer study of bubbles in the dilutor.:	https://www.doi.org/10.1016/j.fluid.2015.01.010
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1251
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107028&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
hf:	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