2-Propyn-1-ol

Other names:	1-Hydroxy-2-propyne
	1-Propyn-3-ol
	1-Propyn-3-yl alcohol
	1-Propyne-3-ol
	2-Propynol
	2-Propynyl alcohol
	2-propyn-1-ol (propargyl alcohol)
	3-Hydroxy-1-propyne
	3-Propynol
	Ethynyl carbinol
	HC«equiv»CCH2OH
	Methanol, ethynyl-
	NSC 8804
	Propynyl alcohol
	Rcra waste number P102
	prop-2-yn-1-ol
	propargyl alcohol
Inchi:	InChI=1S/C3H4O/c1-2-3-4/h1,4H,3H2
InchiKey:	TVDSBUOJIPERQY-UHFFFAOYSA-N
Formula:	C3H4O
SMILES:	C#CCO
Mol. weight [g/mol]:	56.06
CAS:	107-19-7

Physical Properties

Property code	Value	Unit	Source
hfus	10.59	kJ/mol	Joback Method
hvap	49.92	kJ/mol	Cheméo Relay (1.0)
ie	10.50	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
logp	-0.388		Crippen Method
mcvol	50.400	ml/mol	McGowan Method
rinpol	559.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	552.00		NIST Webbook

rinpol	546.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	576.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1357.00		NIST Webbook
tb	387.50 ± 0.50	K	NIST Webbook
tb	386.80	K	NIST Webbook
tb	386.75 ± 0.50	K	NIST Webbook
tb	385.00 ± 3.00	K	NIST Webbook
tf	221.35 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.35	J/mol×K	350.34	Joback Method
cpg	85.08	J/mol×K	379.26	Joback Method
cpg	88.64	J/mol×K	408.19	Joback Method
cpg	92.02	J/mol×K	437.11	Joback Method
cpg	95.25	J/mol×K	466.04	Joback Method
cpg	98.32	J/mol×K	494.96	Joback Method
cpg	101.24	J/mol×K	523.88	Joback Method
hvapt	42.00	kJ/mol	340.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.46079e+01
Coeff. B	-7.44693e+03
Coeff. C	-8.68936e+00
Coeff. D	6.86908e-06
Temperature range (K), min.	221.35
Temperature range (K), max.	580.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-liquid equilibrium study for ternary systems of water + propargyl alcohol + solvents at 303.2 K:	https://www.doi.org/10.1016/j.jct.2019.03.033
Determination of Henry's Law Constants Using Internal Standards Measurement and Thermodynamic Modeling:	https://www.doi.org/10.1021/je3010535
McGowan Method Values:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0, beta):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=894
KDB:	https://www.cheric.org/files/research/kdb/mol/mol894.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Liquid-liquid equilibrium of the ternary system water p propargyl alcohol p n propyl acetate:	https://www.doi.org/10.1016/j.fluid.2016.10.023
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107197&Units=SI
Liquid liquid equilibria of ternary mixture (propargyl alcohol + diisopropyl ether +water):	https://www.doi.org/10.1016/j.fluid.2007.07.015
Liquid-liquid equilibrium of ternary mixture (propargyl alcohol +water + butyl acetate):	https://www.doi.org/10.1016/j.fluid.2009.04.010

Legend

cpg:	Ideal gas heat capacity
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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tf: Normal melting (fusion) point