3-Butyn-2-ol, 2-methyl-

Other names:	1,1-Dimethyl-2-propynol
	1,1-Dimethylpropargyl alcohol
	1,1-Dimethylpropynol
	1-Butyn-3-ol, 3-methyl-
	2-Hydroxy-2-methyl-3-butyne
	2-Methyl-2-butynol
	2-Methyl-3-butyn-2-ol
	2-Methylbutyn-3-ol-2
	2-methylbut-3-yn-2-ol
	3-Hydroxy-3-methyl-1-butyne
	3-Methyl-1-butyn-3-ol
	3-Methyl-butin-(1)-ol-(3)
	3-Methylbutynol
	Carbavane
	Dimethylacetylenecarbinol
	Dimethylacetylenylcarbinol
	Dimethylethynylcarbinol
	Dimethylethynylmethanol
	Ethynyldimethylcarbinol
	NSC 523
	«alpha»,«alpha»-Dimethylpropargyl alcohol
	Â«alphaÂ»,Â«alphaÂ»-Dimethylpropargyl alcohol
Inchi:	InChI=1S/C5H8O/c1-4-5(2,3)6/h1,6H,2-3H3
InchiKey:	CEBKHWWANWSNTI-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C#CC(C)(C)O
Mol. weight [g/mol]:	84.12
CAS:	115-19-5

Physical Properties

Property code	Value	Unit	Source
gf	80.31	kJ/mol	Joback Method
hf	-15.61	kJ/mol	Joback Method
hfus	8.35	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
ie	10.18	eV	NIST Webbook

log10ws	-1.09		Crippen Method
logp	0.390		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
rinpol	544.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	544.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1230.00		NIST Webbook
tb	377.20	K	NIST Webbook
tb	377.00	K	NIST Webbook
tb	377.15 ± 0.50	K	NIST Webbook
tc	577.08	K	Joback Method
tf	275.15 ± 1.50	K	NIST Webbook
tf	276.16 ± 0.20	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.06	J/mol×K	392.87	Joback Method
cpg	154.88	J/mol×K	423.57	Joback Method
cpg	162.21	J/mol×K	454.27	Joback Method
cpg	169.07	J/mol×K	484.97	Joback Method
cpg	175.51	J/mol×K	515.67	Joback Method
cpg	181.53	J/mol×K	546.38	Joback Method
cpg	187.18	J/mol×K	577.08	Joback Method
hvapt	41.00	kJ/mol	355.00	NIST Webbook
hvapt	43.90	kJ/mol	337.00	NIST Webbook
hvapt	49.50	kJ/mol	337.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65055e+01
Coeff. B	-3.93518e+03

Coeff. C	-4.59560e+01
Temperature range (K), min.	288.15
Temperature range (K), max.	397.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115195&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
pc:	Critical Pressure
pvap:	Vapor pressure
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