3-Butyn-2-ol

Other names:	1-Butyn-3-ol
	1-Ethynylethanol
	1-Methyl-2-propynyl alcohol
	1-Methylpropargyl alcohol
	3-Butyne-2-ol
	3-Hydroxy-1-butyne
	HC«equiv»CCH(CH3)OH
	HCÂ«equivÂ»CCH(CH3)OH
	Methylethynylcarbinol
	but-3-yn-2-ol
	«alpha»-Methylpropargyl alcohol
	Â«alphaÂ»-Methylpropargyl alcohol
Inchi:	InChI=1S/C4H6O/c1-3-4(2)5/h1,4-5H,2H3
InchiKey:	GKPOMITUDGXOSB-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	C#CC(C)O
Mol. weight [g/mol]:	70.09
CAS:	2028-63-9

Physical Properties

Property code	Value	Unit	Source
gf	66.61	kJ/mol	Joback Method
hf	8.50	kJ/mol	Joback Method
hfus	9.66	kJ/mol	Joback Method
hvap	40.65	kJ/mol	Joback Method
ie	10.41	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
log10ws	-0.67		Crippen Method
logp	4.000e-04		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
rinpol	608.00		NIST Webbook
rinpol	608.00		NIST Webbook
tb	381.00	K	NIST Webbook
tc	550.21	K	Joback Method
tf	227.63	K	Joback Method
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.88	J/mol×K	372.78	Joback Method
cpg	117.36	J/mol×K	402.35	Joback Method
cpg	122.60	J/mol×K	431.92	Joback Method
cpg	127.58	J/mol×K	461.49	Joback Method
cpg	132.34	J/mol×K	491.06	Joback Method
cpg	136.86	J/mol×K	520.64	Joback Method
cpg	141.18	J/mol×K	550.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65003e+01
Coeff. B	-3.96776e+03
Coeff. C	-4.70680e+01
Temperature range (K), min.	292.15
Temperature range (K), max.	402.15

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2028639&Units=SI

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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume