2-Butyne-1,4-diol

Other names:	1,2-Dimethoxyacetylene
	1,4-BUTYNEDIOL
	1,4-Dihydroxy-2-butyne
	2-Butin-1,4-diol
	2-Butynediol
	2-butyn-1,4-diol
	2-butyne, 1,4-diol-
	BIS(HYDROXYMETHYL)ACETYLENE
	BUTYNEDIOL
	But-2-yne-1,4-diol
	NSC 834
	UN 2716
Inchi:	InChI=1S/C4H6O2/c5-3-1-2-4-6/h5-6H,3-4H2
InchiKey:	DLDJFQGPPSQZKI-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	OCC#CCO
Mol. weight [g/mol]:	86.09
CAS:	110-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-88.04	kJ/mol	Joback Method
hf	-158.05	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	0.18		Crippen Method
logp	-1.026		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	511.20	K	NIST Webbook
tb	511.00	K	NIST Webbook
tc	662.26	K	Joback Method
tf	362.58	K	Joback Method
vc	0.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.52	J/mol×K	484.28	Joback Method
cpg	144.44	J/mol×K	513.94	Joback Method
cpg	149.17	J/mol×K	543.61	Joback Method
cpg	153.72	J/mol×K	573.27	Joback Method
cpg	158.09	J/mol×K	602.94	Joback Method
cpg	162.28	J/mol×K	632.60	Joback Method
cpg	166.30	J/mol×K	662.26	Joback Method
hvapt	81.50	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography
hvapt	69.00	kJ/mol	469.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.00	K	2.00	NIST Webbook
tbrp	418.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76213e+01
Coeff. B	-5.25702e+03
Coeff. C	-1.06705e+02
Temperature range (K), min.	409.99
Temperature range (K), max.	533.96

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.73365e+02
Coeff. B	-1.75313e+04
Coeff. C	-2.18926e+01
Coeff. D	7.85071e-06
Temperature range (K), min.	331.00
Temperature range (K), max.	695.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=913
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor-liquid equilibrium of mixtures containing formaldehyde, water, and methanol:	https://www.doi.org/10.1016/j.fluid.2019.02.029
Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je060333x
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=C110656&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol913.mol

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume