3-Butyn-1-ol

Other names:	1-Butyn-4-ol
	2-Hydroxyethylacetylene
	3-Butyne-1-ol
	3-Butynol
	3-Butynyl alcohol
	4-Hydroxy-1-butyne
	HC«equiv»CCH2CH2OH
	HCÂ«equivÂ»CCH2CH2OH
	NSC 9708
	but-3-yn-1-ol
Inchi:	InChI=1S/C4H6O/c1-2-3-4-5/h1,5H,3-4H2
InchiKey:	OTJZCIYGRUNXTP-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	C#CCCO
Mol. weight [g/mol]:	70.09
CAS:	927-74-2

Physical Properties

Property code	Value	Unit	Source
gf	69.05	kJ/mol	Joback Method
hf	13.78	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	51.70 ± 0.90	kJ/mol	NIST Webbook
ie	9.66	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.002		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
rinpol	660.00		NIST Webbook
tb	402.20	K	NIST Webbook
tb	401.00	K	NIST Webbook
tb	402.05 ± 0.50	K	NIST Webbook
tc	546.50	K	Joback Method
tf	209.55 ± 0.40	K	NIST Webbook
vc	0.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.90	J/mol×K	373.22	Joback Method
cpg	117.17	J/mol×K	402.10	Joback Method
cpg	122.20	J/mol×K	430.98	Joback Method
cpg	127.00	J/mol×K	459.86	Joback Method
cpg	131.58	J/mol×K	488.74	Joback Method
cpg	135.96	J/mol×K	517.62	Joback Method
cpg	140.13	J/mol×K	546.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64754e+01
Coeff. B	-4.13068e+03
Coeff. C	-5.26280e+01
Temperature range (K), min.	308.15
Temperature range (K), max.	422.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C927742&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