2-Butyn-1-ol

Other names:	2-Butyne-1-ol
	2-Butynol
	2-Butynyl alcohol
	But-2-yn-1-ol
	CH3C«equiv»CCH2OH
	CH3CÂ«equivÂ»CCH2OH
Inchi:	InChI=1S/C4H6O/c1-2-3-4-5/h5H,4H2,1H3
InchiKey:	NEEDEQSZOUAJMU-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	CC#CCO
Mol. weight [g/mol]:	70.09
CAS:	764-01-2

Physical Properties

Property code	Value	Unit	Source
gf	48.78	kJ/mol	Joback Method
hf	-5.82	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	43.33	kJ/mol	Joback Method
ie	9.78	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.002		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
tb	415.00	K	NIST Webbook
tb	414.00 ± 2.00	K	NIST Webbook
tb	415.70	K	NIST Webbook
tc	577.58	K	Joback Method
tf	301.76	K	Joback Method
vc	0.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.41	J/mol×K	392.10	Joback Method
cpg	113.75	J/mol×K	423.01	Joback Method
cpg	118.91	J/mol×K	453.93	Joback Method
cpg	123.87	J/mol×K	484.84	Joback Method
cpg	128.66	J/mol×K	515.75	Joback Method
cpg	133.27	J/mol×K	546.67	Joback Method
cpg	137.70	J/mol×K	577.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.00	K	13.30	NIST Webbook
tbrp	325.70	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64585e+01
Coeff. B	-4.25045e+03
Coeff. C	-5.67150e+01
Temperature range (K), min.	319.15
Temperature range (K), max.	438.15

Sources

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=C764012&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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