

2-Butynal

Other names:	1-Formyl-1-propyne But-2-ynal CH ₃ CCCHO Methylacetylaldehyde Tetrolaldehyde
Inchi:	InChI=1S/C4H4O/c1-2-3-4-5/h4H,1H3
InchiKey:	REJPDMLLCDXIOV-UHFFFAOYSA-N
Formula:	C ₄ H ₄ O
SMILES:	CC#CC=O
Mol. weight [g/mol]:	68.07
CAS:	1119-19-3

Physical Properties

Property code	Value	Unit	Source
gf	86.08	kJ/mol	Joback Method
hf	60.83	kJ/mol	Joback Method
hfus	11.53	kJ/mol	Joback Method
hvap	33.37	kJ/mol	Joback Method
ie	10.28	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.25 ± 0.05	eV	NIST Webbook
log10ws	-0.57		Crippen Method
logp	0.209		Crippen Method
mcvol	60.190	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	379.70	K	NIST Webbook
tc	549.03	K	Joback Method
tf	282.94	K	Joback Method
vc	0.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.96	J/mol×K	348.58	Joback Method

cpg	94.79	J/mol×K	381.99	Joback Method
cpg	99.45	J/mol×K	415.40	Joback Method
cpg	103.93	J/mol×K	448.80	Joback Method
cpg	108.24	J/mol×K	482.21	Joback Method
cpg	112.38	J/mol×K	515.62	Joback Method
cpg	116.36	J/mol×K	549.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	300.70	K	4.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38625e+01
Coeff. B	-3.24478e+03
Coeff. C	-4.66930e+01
Temperature range (K), min.	285.72
Temperature range (K), max.	426.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119193&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/ci9903071
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
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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