

2-Butynoic acid

Other names:	1-Propynecarboxylic acid 3-Methylpropionic acid Tetrolic acid
Inchi:	InChI=1S/C4H4O2/c1-2-3-4(5)6/h1H3,(H,5,6)
InchiKey:	LUEHNHVDCZTGL-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	CC#CC(=O)O
Mol. weight [g/mol]:	84.07
CAS:	590-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-80.14	kJ/mol	Joback Method
hf	-118.40	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.094		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	6037.30	kPa	Joback Method
tb	476.20	K	NIST Webbook
tc	643.82	K	Joback Method
tf	351.69	K	Joback Method
vc	0.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.39	J/mol×K	445.97	Joback Method
cpg	120.19	J/mol×K	478.95	Joback Method
cpg	124.79	J/mol×K	511.92	Joback Method
cpg	129.20	J/mol×K	544.90	Joback Method
cpg	133.42	J/mol×K	577.87	Joback Method
cpg	137.46	J/mol×K	610.85	Joback Method

cpg

141.31

J/mol×K

643.82

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.00	K	2.00	NIST Webbook
tbrp	372.70	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56871e+01
Coeff. B	-4.45703e+03
Coeff. C	-7.35340e+01
Temperature range (K), min.	363.15
Temperature range (K), max.	503.15

Sources

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C590932&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
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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