

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:	LUEHNNHVDCZTGL-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
hfus	14.92	kJ/mol	Joback Method
ie	10.36	eV	Cheméo Relay (1.0)
logp	0.094		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
tb	476.20	K	NIST Webbook
tf	364.14	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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=C590932&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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