Propiolic acid

Other names:	2-Propynoic acid
	Acetylenecarboxylic acid
	Carboxyacetylene
	HC«equiv»CCOOH
	HCÂ«equivÂ»CCOOH
	Propargylic acid
	Propinoic acid
	Propynoic acid
Inchi:	InChI=1S/C3H2O2/c1-2-3(4)5/h1H,(H,4,5)
InchiKey:	UORVCLMRJXCDCP-UHFFFAOYSA-N
Formula:	C3H2O2
SMILES:	C#CC(=O)O
Mol. weight [g/mol]:	70.05
CAS:	471-25-0

Physical Properties

Property code	Value	Unit	Source
gf	-68.29	kJ/mol	Joback Method
hf	-78.16	kJ/mol	Joback Method
hfus	12.19	kJ/mol	Joback Method
hvap	45.56	kJ/mol	Joback Method
ie	10.90	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
log10ws	0.03		Crippen Method
logp	-0.296		Crippen Method
mcvol	51.970	ml/mol	McGowan Method
pc	6909.85	kPa	Joback Method
rinpol	660.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1538.00		NIST Webbook
tb	404.21	K	Joback Method
tc	591.76	K	Joback Method
tf	281.29	K	Joback Method
vc	0.191	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.66	J/mol×K	404.21	Joback Method
cpg	89.80	J/mol×K	435.47	Joback Method
cpg	92.76	J/mol×K	466.73	Joback Method
cpg	95.56	J/mol×K	497.98	Joback Method
cpg	98.20	J/mol×K	529.24	Joback Method
cpg	100.69	J/mol×K	560.50	Joback Method
cpg	103.03	J/mol×K	591.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.20	K	26.70	NIST Webbook
tbrp	337.60	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56748e+01
Coeff. B	-4.22610e+03
Coeff. C	-6.56650e+01
Temperature range (K), min.	340.15
Temperature range (K), max.	473.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C471250&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	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