2-Propyn-1-ol, acetate

Other names:	Propargyl acetate
	Propargyl alcohol acetate
	2-Propynyl acetate
	3-Acetoxypropyne
Inchi:	InChI=1S/C5H6O2/c1-3-4-7-5(2)6/h1H,4H2,2H3
InchiKey:	RIZZXCJMFIGMON-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	C#CCOC(C)=O
Mol. weight [g/mol]:	98.10
CAS:	627-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-19.63	kJ/mol	Joback Method
hf	-99.43	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.183		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
rinpol	672.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	395.00 ± 4.00	K	NIST Webbook
tb	397.70	K	NIST Webbook
tb	397.00 ± 4.00	K	NIST Webbook
tc	572.00	K	Joback Method
tf	265.24	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.27	J/mol×K	380.21	Joback Method

cpg	146.80	J/mol×K	412.17	Joback Method
cpg	153.11	J/mol×K	444.14	Joback Method
cpg	159.19	J/mol×K	476.10	Joback Method
cpg	165.05	J/mol×K	508.07	Joback Method
cpg	170.68	J/mol×K	540.03	Joback Method
cpg	176.08	J/mol×K	572.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	301.00	K	1.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627098&Units=SI
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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