1-METHYLALLYL ACETATE

Other names:	1-Methyl-2-propenyl acetate
	3-Buten-2-ol, acetate
	Acetic acid 1-buten-3-yl ester
Inchi:	InChI=1S/C6H10O2/c1-4-5(2)8-6(3)7/h4-5H,1H2,2-3H3
InchiKey:	LYWCPTCPTWCZSZ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=CC(C)OC(C)=O
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
af	0.3340		Cheméo Relay (1.0)
hf	-399.74	kJ/mol	Cheméo Relay (1.0)
hfus	9.28	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.124		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	760.90		NIST Webbook
rinpol	760.90		NIST Webbook
tb	385.70 ± 2.00	K	NIST Webbook
tb	385.00	K	NIST Webbook
tc	542.85	K	Cheméo Relay (1.0)
tf	196.96	K	Cheméo Relay (1.0)
vc	0.359	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.94	J/mol×K	409.21	Joback Method
cpg	194.42	J/mol×K	440.14	Joback Method
cpg	203.56	J/mol×K	471.07	Joback Method

cpg	212.35	J/mol×K	502.00	Joback Method
cpg	220.81	J/mol×K	532.93	Joback Method
cpg	228.92	J/mol×K	563.86	Joback Method
cpg	236.69	J/mol×K	594.78	Joback Method
dvisc	0.0040214	Pa×s	212.78	Joback Method
dvisc	0.0018765	Pa×s	245.52	Joback Method
dvisc	0.0010476	Pa×s	278.26	Joback Method
dvisc	0.0006612	Pa×s	311.00	Joback Method
dvisc	0.0004556	Pa×s	343.73	Joback Method
dvisc	0.0003349	Pa×s	376.47	Joback Method
dvisc	0.0002586	Pa×s	409.21	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6737117&Units=SI

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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume