1-Methylallyl acetate

Other names: Acetic acid 1-buten-3-yl ester
1-Methyl-2-propenyl acetate
3-Buten-2-ol, acetate
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
CAS: 6737-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-148.88	kJ/mol	Joback Method
hf	-291.82	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	37.05	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
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	385.00	K	NIST Webbook
tb	385.70 ± 2.00	K	NIST Webbook
tc	594.78	K	Joback Method
tf	212.78	K	Joback Method
vc	0.370	m3/kmol	Joback Method

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

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume