3-Methyl-3-butenyl acetate

Inchi: InChI=1S/C7H12O2/c1-6(2)4-5-9-7(3)8/h1,4-5H2,2-3H3
InchiKey: OCUAPVNNQFAQSM-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: C=C(C)CCOC(C)=O
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-146.57	kJ/mol	Joback Method
hf	-316.97	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
ripol	1234.00		NIST Webbook
tb	432.41	K	Joback Method
tc	615.89	K	Joback Method
tf	225.09	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.80	J/mol×K	432.41	Joback Method
cpg	233.44	J/mol×K	462.99	Joback Method
cpg	243.68	J/mol×K	493.57	Joback Method
cpg	253.52	J/mol×K	524.15	Joback Method
cpg	262.97	J/mol×K	554.73	Joback Method
cpg	272.04	J/mol×K	585.31	Joback Method
cpg	280.72	J/mol×K	615.89	Joback Method

Sources

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=R600225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume