

3-Methyl-3-buten-1-ol, acetate

Other names:	3-Buten-1-ol, 3-methyl-, acetate Acetic acid, 3-methylbut-3-enyl ester 3-Buten-1-ol, 3-methyl-, 1-acetate 3-Methyl-3-butenyl acetate 1-Acetoxy-3-methyl-3-butene 3-Methyl-3-buten- 1-yl acetate 3-methylbut-3-enyl acetate 3-methylbut-3-en-1-yl 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
CAS:	5205-07-2

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
rinpol	881.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	883.30		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	885.00		NIST Webbook

rinpol	864.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1182.00		NIST Webbook
tb	432.41	K	Joback Method
tc	615.89	K	Joback Method
tf	225.09	K	Joback Method
vc	0.433	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5205072&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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