2-Buten-1-ol, 3-methyl-, acetate

Other names:	3,3-Dimethylallyl acetate
	3-Methyl, but-2-enyl acetate
	3-Methyl-2-buten-1-ol, acetate
	3-Methyl-2-buten-1-yl acetate
	3-Methyl-2-butenyl acetate
	3-Methyl-but-2-en-1-yl acetate
	Dimethylallyl acetate
	Isopent-2-enyl acetate
	Prenyl acetate
	«gamma»,«gamma»-Dimethylallyl acetate
	Â«gammaÂ»,Â«gammaÂ»-Dimethylallyl acetate
Inchi:	InChI=1S/C7H12O2/c1-6(2)4-5-9-7(3)8/h4H,5H2,1-3H3
InchiKey:	XXIKYCPRDXIMQM-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CC(=O)OCC=C(C)C
Mol. weight [g/mol]:	128.17
CAS:	1191-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	917.90		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	902.00		NIST Webbook

rinpol	923.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	917.90		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1248.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1249.00		NIST Webbook
ripol	1254.00		NIST Webbook
tb	439.89	K	Joback Method
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/mol×K	439.89	Joback Method
cpg	233.55	J/mol×K	471.32	Joback Method
cpg	244.02	J/mol×K	502.76	Joback Method
cpg	254.05	J/mol×K	534.19	Joback Method

cpg	263.64	J/mol×K	565.63	Joback Method
cpg	272.80	J/mol×K	597.06	Joback Method
cpg	281.54	J/mol×K	628.49	Joback Method
hvapt	47.80	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.89075e+01
Coeff. B	-5.07474e+03
Coeff. C	-6.56080e+01
Temperature range (K), min.	338.15
Temperature range (K), max.	438.86

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
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=C1191168&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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