1,3-Butadien-1-ol, acetate

Other names:	1-Acetoxy-1,3-butadiene
	Butadienyl acetate
	1-Acetoxybutadiene
	1,3-Butadienyl acetate
	Acetic acid, 1,3-butadienyl ester
	1,3-Butadienylester kyseliny octove
Inchi:	InChI=1S/C6H8O2/c1-3-4-5-8-6(2)7/h3-5H,1H2,2H3/b5-4+
InchiKey:	NMQQBXHZBNUXGJ-SNAWJCMRSA-N
Formula:	C6H8O2
SMILES:	C=CC=COC(C)=O
Mol. weight [g/mol]:	112.13
CAS:	1515-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-66.22	kJ/mol	Joback Method
hf	-169.32	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	37.39	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.249		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	413.81	K	Joback Method
tc	604.45	K	Joback Method
tf	229.10 ± 0.60	K	NIST Webbook
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.29	J/mol×K	413.81	Joback Method
cpg	178.07	J/mol×K	445.58	Joback Method
cpg	186.44	J/mol×K	477.36	Joback Method

cpg	194.43	J/mol×K	509.13	Joback Method
cpg	202.05	J/mol×K	540.91	Joback Method
cpg	209.30	J/mol×K	572.68	Joback Method
cpg	216.19	J/mol×K	604.45	Joback Method
dvisc	0.0024368	Pa×s	222.70	Joback Method
dvisc	0.0012736	Pa×s	254.55	Joback Method
dvisc	0.0007690	Pa×s	286.40	Joback Method
dvisc	0.0005137	Pa×s	318.25	Joback Method
dvisc	0.0003692	Pa×s	350.11	Joback Method
dvisc	0.0002805	Pa×s	381.96	Joback Method
dvisc	0.0002222	Pa×s	413.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	5.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1515760&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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