2-Propene-1,1-diol, diacetate

Other names:	Acrolein, diacetate
	Allylidene acetate
	Allylidene diacetate
	Diacetoxypropene
	Shell SD 345
	SD 345 (Ester)
	SD-345
	1,1-Diacetoxy-2-propene
	Acrolein diacetyl acetal
	Acrolein hydrate diacetate
	Acrolein, monohydrate, diacetate
	Shell 345
	1,1-Diacetoxypropene-2
	3,3-Diacetoxypropene
	2-Propenal, monohydrate, diacetate
	Acetic acid 1-acetoxy-allyl ester
	3,3-Diacetoxy-1-propene
	NSC 45020
	NSC 7632
Inchi:	InChI=1S/C7H10O4/c1-4-7(10-5(2)8)11-6(3)9/h4,7H,1H2,2-3H3
InchiKey:	TXECTBGVEUDNSL-UHFFFAOYSA-N
Formula:	C7H10O4
SMILES:	C=CC(OC(C)=O)OC(C)=O
Mol. weight [g/mol]:	158.15
CAS:	869-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-374.38	kJ/mol	Joback Method
hf	-557.26	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	48.43	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.625		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	457.20	K	NIST Webbook

tc	701.86	K	Joback Method
tf	235.55	K	NIST Webbook
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.65	J/mol×K	508.38	Joback Method
cpg	270.66	J/mol×K	540.63	Joback Method
cpg	280.29	J/mol×K	572.87	Joback Method
cpg	289.53	J/mol×K	605.12	Joback Method
cpg	298.36	J/mol×K	637.37	Joback Method
cpg	306.78	J/mol×K	669.62	Joback Method
cpg	314.78	J/mol×K	701.86	Joback Method
dvisc	0.0025417	Pa×s	296.21	Joback Method
dvisc	0.0013888	Pa×s	331.57	Joback Method
dvisc	0.0008526	Pa×s	366.93	Joback Method
dvisc	0.0005703	Pa×s	402.30	Joback Method
dvisc	0.0004070	Pa×s	437.66	Joback Method
dvisc	0.0003056	Pa×s	473.02	Joback Method
dvisc	0.0002387	Pa×s	508.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C869294&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume