

2-Propene-1,1-diol, 2-methyl-, diacetate

Other names:	Methacrolein diacetate Methallylidene diacetate Acetic acid, 2-methyl-2-propene-1,1-diol diester 2-Methyl-2-propene-1,1-diol diacetate 2-methylallylidene diacetate
Inchi:	InChI=1S/C8H12O4/c1-5(2)8(11-6(3)9)12-7(4)10/h8H,1H2,2-4H3
InchiKey:	QFXJBPCTHSTOPE-UHFFFAOYSA-N
Formula:	C8H12O4
SMILES:	C=C(C)C(OC(C)=O)OC(C)=O
Mol. weight [g/mol]:	172.18
CAS:	10476-95-6

Physical Properties

Property code	Value	Unit	Source
gf	-374.51	kJ/mol	Joback Method
hf	-587.69	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	50.74	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.015		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	464.20	K	NIST Webbook
tc	725.59	K	Joback Method
tf	293.52	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.63	J/molxK	531.14	Joback Method
cpg	314.89	J/molxK	563.55	Joback Method
cpg	325.67	J/molxK	595.96	Joback Method
cpg	335.99	J/molxK	628.37	Joback Method

cpg	345.83	J/mol×K	660.77	Joback Method
cpg	355.18	J/mol×K	693.18	Joback Method
cpg	364.05	J/mol×K	725.59	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=C10476956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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