

Dimethyl(E)-1-propenyl orthoacetate

Inchi:	InChI=1S/C7H14O3/c1-5-6-10-7(2,8-3)9-4/h5-6H,1-4H3/b6-5+
InchiKey:	XJZFAGYWNJDGRK-AATRIKPKSA-N
Formula:	C7H14O3
SMILES:	CC=COC(C)(OC)OC
Mol. weight [g/mol]:	146.18
CAS:	66178-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-223.88	kJ/mol	Joback Method
hf	-476.00	kJ/mol	Joback Method
hfus	10.24	kJ/mol	Joback Method
hvap	37.07	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.503		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	427.75	K	Joback Method
tc	611.93	K	Joback Method
tf	232.68	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.70	J/mol×K	427.75	Joback Method
cpg	308.53	J/mol×K	581.23	Joback Method
cpg	298.26	J/mol×K	550.54	Joback Method
cpg	287.55	J/mol×K	519.84	Joback Method
cpg	276.39	J/mol×K	489.14	Joback Method
cpg	264.77	J/mol×K	458.45	Joback Method
cpg	318.36	J/mol×K	611.93	Joback Method
dvisc	0.0001510	Pa×s	427.75	Joback Method
dvisc	0.0002035	Pa×s	395.24	Joback Method

dvisc	0.0002894	Pa×s	362.73	Joback Method
dvisc	0.0004411	Pa×s	330.22	Joback Method
dvisc	0.0007371	Pa×s	297.70	Joback Method
dvisc	0.0013970	Pa×s	265.19	Joback Method
dvisc	0.0031657	Pa×s	232.68	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66178210&Units=SI

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

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