(E,Z) Di-1-propenyl methyl orthoacetate

Inchi: InChI=1S/C9H16O3/c1-5-7-11-9(3,10-4)12-8-6-2/h5-8H,1-4H3/b7-5-,8-6+
InchiKey: OKCRPXLGUMMWRB-CGXWXWIYSA-N
Formula: C9H16O3
SMILES: CC=COC(C)(OC)OC=CC
Mol. weight [g/mol]: 172.22
CAS: 66178-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-126.82	kJ/mol	Joback Method
hf	-400.06	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.407		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	477.67	K	Joback Method
tc	667.08	K	Joback Method
tf	250.14	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.22	J/mol×K	477.67	Joback Method
cpg	334.14	J/mol×K	509.24	Joback Method
cpg	347.41	J/mol×K	540.81	Joback Method
cpg	360.06	J/mol×K	572.37	Joback Method
cpg	372.11	J/mol×K	603.94	Joback Method
cpg	383.57	J/mol×K	635.51	Joback Method
cpg	394.46	J/mol×K	667.08	Joback Method
dvisc	0.0027854	Pa×s	250.14	Joback Method
dvisc	0.0011283	Pa×s	288.06	Joback Method

dvisc	0.0005640	Pa×s	325.98	Joback Method
dvisc	0.0003257	Pa×s	363.90	Joback Method
dvisc	0.0002087	Pa×s	401.83	Joback Method
dvisc	0.0001443	Pa×s	439.75	Joback Method
dvisc	0.0001059	Pa×s	477.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66178243&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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