

(E,E) 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-KQQUZDAGSA-N
Formula:	C9H16O3
SMILES:	CC=COC(C)(OC)OC=CC
Mol. weight [g/mol]:	172.22
CAS:	66178-23-2

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/molxK	477.67	Joback Method
cpg	383.57	J/molxK	635.51	Joback Method
cpg	372.11	J/molxK	603.94	Joback Method
cpg	360.06	J/molxK	572.37	Joback Method
cpg	347.41	J/molxK	540.81	Joback Method
cpg	334.14	J/molxK	509.24	Joback Method
cpg	394.46	J/molxK	667.08	Joback Method
dvisc	0.0001059	Paxs	477.67	Joback Method
dvisc	0.0001443	Paxs	439.75	Joback Method

dvisc	0.0002087	Paxs	401.83	Joback Method
dvisc	0.0003257	Paxs	363.90	Joback Method
dvisc	0.0005640	Paxs	325.98	Joback Method
dvisc	0.0011283	Paxs	288.06	Joback Method
dvisc	0.0027854	Paxs	250.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C66178232&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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