Acrolein,dimethyl acetal

Other names: 1-Propene, 3,3-dimethoxy-
3,3-Dimethoxypropene-1
3,3-dimethoxypropene
Inchi: InChI=1S/C5H10O2/c1-4-5(6-2)7-3/h4-5H,1H2,2-3H3
InchiKey: OBWGMYALGNDUNM-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: C=CC(OC)OC
Mol. weight [g/mol]: 102.13
CAS: 6044-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-133.38	kJ/mol	Joback Method
hf	-290.82	kJ/mol	Joback Method
hfus	6.28	kJ/mol	Joback Method
hvap	30.49	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.791		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	668.00		NIST Webbook
tb	362.70	K	NIST Webbook
tc	527.84	K	Joback Method
tf	173.81	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.17	J/mol×K	354.88	Joback Method
cpg	164.28	J/mol×K	383.71	Joback Method
cpg	172.23	J/mol×K	412.53	Joback Method
cpg	179.99	J/mol×K	441.36	Joback Method
cpg	187.57	J/mol×K	470.18	Joback Method

cpg	194.96	J/mol×K	499.01	Joback Method
cpg	202.16	J/mol×K	527.84	Joback Method
dvisc	0.0035623	Pa×s	173.81	Joback Method
dvisc	0.0015233	Pa×s	203.99	Joback Method
dvisc	0.0008108	Pa×s	234.17	Joback Method
dvisc	0.0004984	Pa×s	264.35	Joback Method
dvisc	0.0003385	Pa×s	294.52	Joback Method
dvisc	0.0002471	Pa×s	324.70	Joback Method
dvisc	0.0001902	Pa×s	354.88	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=C6044684&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume