Acrolein, 3-ethoxy-, diethyl acetal

Other names:	Propene, 1,3,3-triethoxy- 1-Propene, 1,3,3-triethoxy- 1,3,3-Triethoxy-1-propene 1,3,3-Triethoxypropene «beta»-Ethoxyacroleindiethylacetal
Inchi:	InChI=1S/C9H18O3/c1-4-10-8-7-9(11-5-2)12-6-3/h7-9H,4-6H2,1-3H3/b8-7+
InchiKey:	ATAQLIDYIFWHFW-BQYQJAHWSA-N
Formula:	C9H18O3
SMILES:	CCOC=CC(OCC)OCC
Mol. weight [g/mol]:	174.24
CAS:	5444-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-212.32	kJ/mol	Joback Method
hf	-513.81	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	42.43	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.936		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	476.30	K	Joback Method
tc	650.52	K	Joback Method
tf	237.80	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.25	J/mol×K	476.30	Joback Method
cpg	397.29	J/mol×K	621.48	Joback Method

cpg	385.55	J/mol×K	592.45	Joback Method
cpg	373.37	J/mol×K	563.41	Joback Method
cpg	360.76	J/mol×K	534.37	Joback Method
cpg	347.72	J/mol×K	505.34	Joback Method
cpg	408.60	J/mol×K	650.52	Joback Method
dvisc	0.0001208	Pa×s	476.30	Joback Method
dvisc	0.0001621	Pa×s	436.55	Joback Method
dvisc	0.0002308	Pa×s	396.80	Joback Method
dvisc	0.0003553	Pa×s	357.05	Joback Method
dvisc	0.0006096	Pa×s	317.30	Joback Method
dvisc	0.0012205	Pa×s	277.55	Joback Method
dvisc	0.0030823	Pa×s	237.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5444804&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume