1-Propene, 3,3-diethoxy-

Other names:	Acrolein, diethyl acetal
	Acrolein acetal
	Acrylaldehyde diethyl acetal
	Propenal diethyl acetal
	1,1-Diethoxy-2-propene
	3,3-Diethoxypropene
	UN 2374
	3,3-Diethoxy-1-propene
	NSC 60135
Inchi:	InChI=1S/C7H14O2/c1-4-7(8-5-2)9-6-3/h4,7H,1,5-6H2,2-3H3
InchiKey:	MCIPQLOKVXSHTD-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	C=CC(OCC)OCC
Mol. weight [g/mol]:	130.18
CAS:	3054-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-116.54	kJ/mol	Joback Method
hf	-332.10	kJ/mol	Joback Method
hfus	11.46	kJ/mol	Joback Method
hvap	34.94	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.571		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	780.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	780.00		NIST Webbook
tb	396.70	K	NIST Webbook
tb	398.20	K	NIST Webbook
tc	572.64	K	Joback Method
tf	196.35	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.34	J/mol×K	400.64	Joback Method
cpg	238.35	J/mol×K	429.31	Joback Method
cpg	249.05	J/mol×K	457.97	Joback Method
cpg	259.44	J/mol×K	486.64	Joback Method
cpg	269.51	J/mol×K	515.31	Joback Method
cpg	279.27	J/mol×K	543.97	Joback Method
cpg	288.70	J/mol×K	572.64	Joback Method
dvisc	0.0041165	Pa×s	196.35	Joback Method
dvisc	0.0016855	Pa×s	230.40	Joback Method
dvisc	0.0008686	Pa×s	264.45	Joback Method
dvisc	0.0005207	Pa×s	298.50	Joback Method
dvisc	0.0003466	Pa×s	332.54	Joback Method
dvisc	0.0002488	Pa×s	366.59	Joback Method
dvisc	0.0001890	Pa×s	400.64	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=C3054953&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