«beta»-Chloropropionaldehyde diethyl acetal

Other names:	3-Chloro-1,1-diethoxypropane
	Propane, 3-chloro-1,1-diethoxy-
	3-Chloropropionaldehyde diethyl acetal
	Propionaldehyde, 3-chloro-, diethyl acetal
Inchi:	InChI=1S/C7H15ClO2/c1-3-9-7(5-6-8)10-4-2/h7H,3-6H2,1-2H3
InchiKey:	NXHONHDWVLPPCS-UHFFFAOYSA-N
Formula:	C7H15ClO2
SMILES:	CCOC(CCCl)OCC
Mol. weight [g/mol]:	166.65
CAS:	35573-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-216.31	kJ/mol	Joback Method
hf	-473.27	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	39.99	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	2.014		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
tb	441.39	K	Joback Method
tc	616.85	K	Joback Method
tf	228.03	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.37	J/mol×K	441.39	Joback Method
cpg	324.29	J/mol×K	587.61	Joback Method
cpg	314.21	J/mol×K	558.36	Joback Method
cpg	303.77	J/mol×K	529.12	Joback Method
cpg	292.98	J/mol×K	499.88	Joback Method

cpg	281.85	J/mol×K	470.63	Joback Method
cpg	334.02	J/mol×K	616.85	Joback Method
dvisc	0.0002044	Pa×s	441.39	Joback Method
dvisc	0.0002711	Pa×s	405.83	Joback Method
dvisc	0.0003796	Pa×s	370.27	Joback Method
dvisc	0.0005711	Pa×s	334.71	Joback Method
dvisc	0.0009465	Pa×s	299.15	Joback Method
dvisc	0.0017981	Pa×s	263.59	Joback Method
dvisc	0.0041725	Pa×s	228.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	3.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35573934&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume