Ethyl 3,3-diethoxypropionate

Other names:	Propanoic acid, 3,3-diethoxy-, ethyl ester
	Ethyl 3,3-diethoxypropanoate
Inchi:	InChI=1S/C9H18O4/c1-4-11-8(10)7-9(12-5-2)13-6-3/h9H,4-7H2,1-3H3
InchiKey:	SIALOQYKFQEKOG-UHFFFAOYSA-N
Formula:	C9H18O4
SMILES:	CCOC(=O)CC(OCC)OCC
Mol. weight [g/mol]:	190.24
CAS:	10601-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-421.46	kJ/mol	Joback Method
hf	-743.61	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.339		Crippen Method
mcvol	156.850	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1163.00		NIST Webbook
tb	526.01	K	Joback Method
tc	701.99	K	Joback Method
tf	292.81	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.48	J/mol×K	526.01	Joback Method
cpg	386.74	J/mol×K	555.34	Joback Method
cpg	399.56	J/mol×K	584.67	Joback Method
cpg	411.95	J/mol×K	614.00	Joback Method
cpg	423.90	J/mol×K	643.33	Joback Method
cpg	435.38	J/mol×K	672.66	Joback Method

cpg	446.38	J/mol×K	701.99	Joback Method
dvisc	0.0023519	Pa×s	292.81	Joback Method
dvisc	0.0011407	Pa×s	331.68	Joback Method
dvisc	0.0006439	Pa×s	370.54	Joback Method
dvisc	0.0004052	Pa×s	409.41	Joback Method
dvisc	0.0002763	Pa×s	448.28	Joback Method
dvisc	0.0002002	Pa×s	487.14	Joback Method
dvisc	0.0001522	Pa×s	526.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	1.70	NIST Webbook

Sources

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=C10601806&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume