2,3-Diethoxy-propionic acid, ethyl ester

Other names:	Ethyl 2,3-diethoxy propionate
	Ethyl 2,3-diethoxypropanoate
Inchi:	InChI=1S/C9H18O4/c1-4-11-7-8(12-5-2)9(10)13-6-3/h8H,4-7H2,1-3H3
InchiKey:	YZLFCKHEPNGJND-UHFFFAOYSA-N
Formula:	C9H18O4
SMILES:	CCOCC(OCC)C(=O)OCC
Mol. weight [g/mol]:	190.24
CAS:	10120-24-8

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	-0.74		Crippen Method
logp	0.991		Crippen Method
mcvol	156.850	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1332.00		NIST Webbook
ripol	1829.00		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

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=C10120248&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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