Ethyl 2,2-diethoxypropionate

Other names: Propanoic acid, 2,2-diethoxy-, ethyl ester
Propionic acid, 2,2-diethoxy-, ethyl ester
Ethyl 2,2-diethoxypropanoate
Inchi: InChI=1S/C9H18O4/c1-5-11-8(10)9(4,12-6-2)13-7-3/h5-7H2,1-4H3
InchiKey: BVAMIFTXHAJQHP-UHFFFAOYSA-N
Formula: C9H18O4
SMILES: CCOC(=O)C(C)(OCC)OCC
Mol. weight [g/mol]: 190.24
CAS: 7476-20-2

Physical Properties

Property code	Value	Unit	Source
gf	-416.18	kJ/mol	Joback Method
hf	-747.08	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	48.31	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.339		Crippen Method
mcvol	156.850	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
tb	523.22	K	Joback Method
tc	705.56	K	Joback Method
tf	310.23	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.37	J/mol×K	523.22	Joback Method
cpg	390.18	J/mol×K	553.61	Joback Method
cpg	403.44	J/mol×K	584.00	Joback Method
cpg	416.15	J/mol×K	614.39	Joback Method

cpg	428.32	J/mol×K	644.78	Joback Method
cpg	439.94	J/mol×K	675.17	Joback Method
cpg	451.01	J/mol×K	705.56	Joback Method
dvisc	0.0021424	Pa×s	310.23	Joback Method
dvisc	0.0011012	Pa×s	345.73	Joback Method
dvisc	0.0006407	Pa×s	381.23	Joback Method
dvisc	0.0004088	Pa×s	416.73	Joback Method
dvisc	0.0002799	Pa×s	452.22	Joback Method
dvisc	0.0002025	Pa×s	487.72	Joback Method
dvisc	0.0001531	Pa×s	523.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.50 ± 0.50	K	3.50	NIST Webbook

Sources

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=C7476202&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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