Acetic acid, ethoxy-, ethyl ester

Other names:	Ethoxyacetic acid ethyl ester
	Ethyl ethoxyacetate
	Ethyl 2-ethoxyacetate
	EThyl ester of ethoxyacetic acid
Inchi:	InChI=1S/C6H12O3/c1-3-8-5-6(7)9-4-2/h3-5H2,1-2H3
InchiKey:	CKSRFHWWBKRUKA-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCOCC(=O)OCC
Mol. weight [g/mol]:	132.16
CAS:	817-95-8

Physical Properties

Property code	Value	Unit	Source
chl	-3436.50 ± 0.60	kJ/mol	NIST Webbook
gf	-339.28	kJ/mol	Joback Method
hf	-544.19	kJ/mol	Joback Method
hfl	-639.50 ± 0.60	kJ/mol	NIST Webbook
hfus	15.27	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.586		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	435.39	K	Joback Method
tc	612.77	K	Joback Method
tf	251.77	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.12	J/mol×K	612.77	Joback Method
cpg	267.77	J/mol×K	583.20	Joback Method
cpg	259.12	J/mol×K	553.64	Joback Method

cpg	250.20	J/mol×K	524.08	Joback Method
cpg	241.01	J/mol×K	494.52	Joback Method
cpg	231.56	J/mol×K	464.95	Joback Method
cpg	221.86	J/mol×K	435.39	Joback Method
dvisc	0.0023571	Pa×s	251.77	Joback Method
dvisc	0.0002392	Pa×s	435.39	Joback Method
dvisc	0.0003033	Pa×s	404.79	Joback Method
dvisc	0.0003996	Pa×s	374.18	Joback Method
dvisc	0.0005532	Pa×s	343.58	Joback Method
dvisc	0.0008159	Pa×s	312.98	Joback Method
dvisc	0.0013093	Pa×s	282.37	Joback Method
hvapt	46.10	kJ/mol	380.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.50 ± 0.50	K	2.40	NIST Webbook

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=C817958&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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