Propanoic acid, 2-oxo-, ethyl ester

Other names:	Pyruvic acid, ethyl ester
	Ethyl pyruvate
	Ethyl 2-oxopropanoate
	Ethyl 2-oxopropionate
Inchi:	InChI=1S/C5H8O3/c1-3-8-5(7)4(2)6/h3H2,1-2H3
InchiKey:	XXRCUYVCPSWGCC-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	CCOC(=O)C(C)=O
Mol. weight [g/mol]:	116.12
CAS:	617-35-6

Physical Properties

Property code	Value	Unit	Source
gf	-371.62	kJ/mol	Joback Method
hf	-503.91	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.138		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	774.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1252.00		NIST Webbook

ripol	1267.00		NIST Webbook
ripol	1234.00		NIST Webbook
tb	428.70 ± 0.80	K	NIST Webbook
tb	417.20	K	NIST Webbook
tb	428.20	K	NIST Webbook
tc	634.74	K	Joback Method
tf	268.20	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.41	J/mol×K	443.96	Joback Method
cpg	213.74	J/mol×K	602.95	Joback Method
cpg	206.83	J/mol×K	571.15	Joback Method
cpg	199.65	J/mol×K	539.35	Joback Method
cpg	192.17	J/mol×K	507.55	Joback Method
cpg	184.43	J/mol×K	475.76	Joback Method
cpg	220.34	J/mol×K	634.74	Joback Method
dvisc	0.0003266	Pa×s	443.96	Joback Method
dvisc	0.0004079	Pa×s	414.67	Joback Method
dvisc	0.0005268	Pa×s	385.37	Joback Method
dvisc	0.0007096	Pa×s	356.08	Joback Method
dvisc	0.0010084	Pa×s	326.79	Joback Method
dvisc	0.0015356	Pa×s	297.49	Joback Method
dvisc	0.0025634	Pa×s	268.20	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C617356&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
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