Propanoic acid, 2-oxo-, methyl ester

Other names:	2-oxopropanoic acid, methyl ester
	Methylglyoxylic acid methyl ester
	methyl 2-oxopropanoate
	methyl pyruvate
	pyruvic acid, methyl ester
Inchi:	InChI=1S/C4H6O3/c1-3(5)4(6)7-2/h1-2H3
InchiKey:	CWKLZLBVOJRSOM-UHFFFAOYSA-N
Formula:	C4H6O3
SMILES:	COC(=O)C(C)=O
Mol. weight [g/mol]:	102.09
CAS:	600-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-380.04	kJ/mol	Joback Method
hf	-483.27	kJ/mol	Joback Method
hfus	10.50	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
ie	9.88	eV	NIST Webbook
log10ws	0.36		Crippen Method
logp	-0.252		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
rinpol	710.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	701.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1217.00		NIST Webbook
tb	408.70	K	NIST Webbook
tb	410.70 ± 0.60	K	NIST Webbook
tb	411.00 ± 6.00	K	NIST Webbook
tc	613.71	K	Joback Method

tf	256.93	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.13	J/mol×K	421.08	Joback Method
cpg	146.68	J/mol×K	453.18	Joback Method
cpg	153.04	J/mol×K	485.29	Joback Method
cpg	159.19	J/mol×K	517.39	Joback Method
cpg	165.13	J/mol×K	549.50	Joback Method
cpg	170.85	J/mol×K	581.60	Joback Method
cpg	176.35	J/mol×K	613.71	Joback Method
dvisc	0.0023950	Pa×s	256.93	Joback Method
dvisc	0.0014709	Pa×s	284.29	Joback Method
dvisc	0.0009841	Pa×s	311.65	Joback Method
dvisc	0.0007025	Pa×s	339.00	Joback Method
dvisc	0.0005274	Pa×s	366.36	Joback Method
dvisc	0.0004120	Pa×s	393.72	Joback Method
dvisc	0.0003324	Pa×s	421.08	Joback Method
pvap	0.18	kPa	279.40	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.17	kPa	279.40	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.19	kPa	280.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.23	kPa	282.40	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.25	kPa	283.80	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.30	kPa	286.20	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.29	kPa	286.20	Thermodynamic properties of pyruvic acid and its methyl ester

pvap	0.30	kPa	287.00	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.36	kPa	289.20	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.43	kPa	291.00	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.53	kPa	294.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.71	kPa	298.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	0.92	kPa	302.90	Thermodynamic properties of pyruvic acid and its methyl ester
pvap	1.23	kPa	307.80	Thermodynamic properties of pyruvic acid and its methyl ester

Sources

Thermodynamic properties of pyruvic acid and its methyl ester:	https://www.doi.org/10.1016/j.tca.2018.05.009
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=C600226&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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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