Methylmalonic acid

Other names:	1,1-Ethanedicarboxylic acid
	2-Methylmalonic acid
	Isosuccinic acid
	Malonic acid, methyl-
	Propanedioic acid, methyl-
Inchi:	InChI=1S/C4H6O4/c1-2(3(5)6)4(7)8/h2H,1H3,(H,5,6)(H,7,8)
InchiKey:	ZIYVHBGGAOATLY-UHFFFAOYSA-N
Formula:	C4H6O4
SMILES:	CC(C(=O)O)C(=O)O
Mol. weight [g/mol]:	118.09
CAS:	516-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-551.12	kJ/mol	Joback Method
hf	-660.79	kJ/mol	Joback Method
hfus	13.97	kJ/mol	Joback Method
hsub	117.40 ± 1.90	kJ/mol	NIST Webbook
hsub	113.20 ± 0.40	kJ/mol	NIST Webbook
hvap	70.96	kJ/mol	Joback Method
ie	10.80	eV	NIST Webbook
log10ws	0.55		Crippen Method
logp	-0.208		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	6065.55	kPa	Joback Method
tb	582.58	K	Joback Method
tc	761.63	K	Joback Method
tf	341.34	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.50	J/mol×K	582.58	Joback Method

cpg	213.48	J/mol×K	731.79	Joback Method
cpg	209.20	J/mol×K	701.95	Joback Method
cpg	204.67	J/mol×K	672.10	Joback Method
cpg	199.88	J/mol×K	642.26	Joback Method
cpg	194.82	J/mol×K	612.42	Joback Method
cpg	217.51	J/mol×K	761.63	Joback Method
dvisc	0.0000564	Pa×s	582.58	Joback Method
dvisc	0.0001019	Pa×s	542.37	Joback Method
dvisc	0.0002027	Pa×s	502.17	Joback Method
dvisc	0.0004543	Pa×s	461.96	Joback Method
dvisc	0.0011876	Pa×s	421.75	Joback Method
dvisc	0.0038013	Pa×s	381.55	Joback Method
dvisc	0.0160048	Pa×s	341.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.44133e+01
Coeff. B	-8.71788e+03
Coeff. C	-1.05448e+02
Temperature range (K), min.	466.80
Temperature range (K), max.	561.84

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=C516052&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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