Ethanedioic acid, dimethyl ester

Other names:	CH3OCOCOOCH3
	DIMETHYL ESTER OXALIC ACID
	DIMETHYL OXALATE
	Dimethyl ester of oxalic acid
	Ethanedioc acid dimethyl ester
	METHYL OXALATE
	Oxalic acid, dimethyl ester
	dimethyl ethanedioate
Inchi:	InChI=1S/C4H6O4/c1-7-3(5)4(6)8-2/h1-2H3
InchiKey:	LOMVENUNSWAXEN-UHFFFAOYSA-N
Formula:	C4H6O4
SMILES:	COC(=O)C(=O)OC
Mol. weight [g/mol]:	118.09
CAS:	553-90-2

Physical Properties

Property code	Value	Unit	Source
af	0.5560		KDB
chs	-1675.20 ± 0.63	kJ/mol	NIST Webbook
chs	-1677.00	kJ/mol	NIST Webbook
gf	-485.04	kJ/mol	Joback Method
hf	-709.70	kJ/mol	NIST Webbook
hf	-709.27 ± 0.54	kJ/mol	NIST Webbook
hfs	-756.73 ± 0.31	kJ/mol	NIST Webbook
hfs	-756.30 ± 0.84	kJ/mol	NIST Webbook
hfus	11.69	kJ/mol	Joback Method
hsub	74.60 ± 0.70	kJ/mol	NIST Webbook
hsub	75.20 ± 0.50	kJ/mol	NIST Webbook
hsub	47.00	kJ/mol	NIST Webbook
hsub	75.30 ± 1.60	kJ/mol	NIST Webbook
hvap	54.70 ± 0.30	kJ/mol	NIST Webbook
hvap	52.50	kJ/mol	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
log10ws	0.78		Crippen Method
logp	-0.668		Crippen Method
mcvol	82.100	ml/mol	McGowan Method

pc	3980.00 ± 405.30	kPa	NIST Webbook
pc	9610.00 ± 2026.50	kPa	NIST Webbook
pc	4060.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
pc	3980.00	kPa	KDB
rinpol	826.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	819.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1409.00		NIST Webbook
tb	437.40 ± 0.50	K	NIST Webbook
tb	437.70	K	NIST Webbook
tb	436.65	K	Determination of Ternary Vapor-Liquid Equilibrium of Dimethyl Oxalate-Methanol-1,2-Butanediol under Atmosphere Pressure
tb	436.50	K	KDB
tb	437.40 ± 0.50	K	NIST Webbook
tc	628.00	K	KDB
tc	533.00 ± 40.00	K	NIST Webbook
tc	628.00 ± 8.00	K	NIST Webbook
tc	533.00 ± 40.00	K	NIST Webbook
tf	322.65 ± 0.60	K	NIST Webbook
tf	327.95 ± 0.25	K	NIST Webbook
tf	327.00	K	KDB
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.25	J/mol×K	443.50	Joback Method
cpg	165.77	J/mol×K	475.48	Joback Method
cpg	172.16	J/mol×K	507.47	Joback Method
cpg	178.40	J/mol×K	539.45	Joback Method
cpg	184.47	J/mol×K	571.43	Joback Method
cpg	190.35	J/mol×K	603.41	Joback Method
cpg	196.03	J/mol×K	635.40	Joback Method
dvisc	0.0002944	Pa×s	443.50	Joback Method
dvisc	0.0012352	Pa×s	306.55	Joback Method
dvisc	0.0008440	Pa×s	333.94	Joback Method
dvisc	0.0006109	Pa×s	361.33	Joback Method
dvisc	0.0019482	Pa×s	279.16	Joback Method
dvisc	0.0003637	Pa×s	416.11	Joback Method
dvisc	0.0004628	Pa×s	388.72	Joback Method
hfust	21.07	kJ/mol	327.60	NIST Webbook
hfust	21.07	kJ/mol	327.60	NIST Webbook
hsubt	75.60 ± 1.60	kJ/mol	283.00	NIST Webbook
hsubt	47.40 ± 0.46	kJ/mol	289.21	NIST Webbook
hvapt	44.70	kJ/mol	416.00	NIST Webbook
hvapt	48.80	kJ/mol	365.00	NIST Webbook
pvap	101.33	kPa	436.65	Determination of Ternary Vapor-Liquid Equilibrium of Dimethyl Oxalate-Methanol-1,2-Butanediol under Atmosphere Pressure
rhol	1150.00	kg/m3	288.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71121e+01
Coeff. B	-5.28130e+03

Coeff. C	-1.49840e+01
Temperature range (K), min.	323.65
Temperature range (K), max.	462.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.59206e+01
Coeff. B	-6.60112e+03
Coeff. C	-2.71833e+00
Coeff. D	1.79251e-06
Temperature range (K), min.	293.15
Temperature range (K), max.	436.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1057
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1057
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C553902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je0602418
Determination of Ternary Vapor-Liquid Equilibrium of Dimethyl Oxalate-Methanol-1,2-Butanediol under Atmosphere Pressure:	https://www.doi.org/10.1021/acs.jced.8b00918
Fedors Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	Liquid Density
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