Propanedioic acid, dimethyl ester

Other names:	1,3-propanedioic acid, dimethyl ester
	Dimethyl ester of malonic acid
	Dimethyl malonate
	Dimethyl propanedioate
	Malonic acid, dimethyl ester
	Methyl malonate
	dimethyl 1,3-propanedioate
Inchi:	InChI=1S/C5H8O4/c1-8-4(6)3-5(7)9-2/h3H2,1-2H3
InchiKey:	BEPAFCGSDWSTEL-UHFFFAOYSA-N
Formula:	C5H8O4
SMILES:	COC(=O)CC(=O)OC
Mol. weight [g/mol]:	132.11
CAS:	108-59-8

Physical Properties

Property code	Value	Unit	Source
chl	-2311.20 ± 0.63	kJ/mol	NIST Webbook
chl	-2311.20 ± 0.63	kJ/mol	NIST Webbook
chs	-2318.00	kJ/mol	NIST Webbook
gf	-476.62	kJ/mol	Joback Method
hf	-737.80 ± 1.00	kJ/mol	NIST Webbook
hf	-737.80 ± 1.00	kJ/mol	NIST Webbook
hfl	-799.69 ± 0.63	kJ/mol	NIST Webbook
hfl	-799.69 ± 0.63	kJ/mol	NIST Webbook
hfus	14.28	kJ/mol	Joback Method
hsub	111.70 ± 2.10	kJ/mol	NIST Webbook
hvap	57.50 ± 0.30	kJ/mol	NIST Webbook
hvap	61.90	kJ/mol	NIST Webbook
hvap	61.84 ± 0.79	kJ/mol	NIST Webbook
hvap	61.84 ± 0.79	kJ/mol	NIST Webbook
log10ws	0.36		Crippen Method
logp	-0.278		Crippen Method
mcvol	96.190	ml/mol	McGowan Method

pc	3530.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
rinpol	917.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	915.00		NIST Webbook
ripol	1506.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1482.00		NIST Webbook
tb	454.60 ± 0.80	K	NIST Webbook
tb	454.60 ± 0.50	K	NIST Webbook
tb	454.60	K	NIST Webbook
tc	656.26	K	Joback Method
tf	211.30 ± 1.00	K	NIST Webbook

vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.70	J/mol×K	466.38	Joback Method
cpg	204.67	J/mol×K	498.03	Joback Method
cpg	212.42	J/mol×K	529.67	Joback Method
cpg	219.95	J/mol×K	561.32	Joback Method
cpg	227.23	J/mol×K	592.97	Joback Method
cpg	234.25	J/mol×K	624.62	Joback Method
cpg	240.99	J/mol×K	656.26	Joback Method
cpl	210.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0002822	Pa×s	466.38	Joback Method
dvisc	0.0012551	Pa×s	319.75	Joback Method
dvisc	0.0020268	Pa×s	290.43	Joback Method
dvisc	0.0006014	Pa×s	378.40	Joback Method
dvisc	0.0004507	Pa×s	407.73	Joback Method
dvisc	0.0003511	Pa×s	437.06	Joback Method
dvisc	0.0008423	Pa×s	349.08	Joback Method
hvapt	52.90 ± 0.20	kJ/mol	405.50	NIST Webbook
hvapt	49.50 ± 0.20	kJ/mol	405.50	NIST Webbook
hvapt	46.10 ± 0.30	kJ/mol	405.50	NIST Webbook
hvapt	61.80 ± 0.80	kJ/mol	293.00	NIST Webbook
hvapt	50.00	kJ/mol	497.00	NIST Webbook
hvapt	53.70	kJ/mol	381.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69518e+01
Coeff. B	-5.19477e+03
Coeff. C	-3.34050e+01
Temperature range (K), min.	345.14
Temperature range (K), max.	479.68

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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=C108598&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hsub:	Enthalpy of sublimation 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
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

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