2-Butenedioic acid (Z)-, dimethyl ester

Other names:	2-BUTENEDIOIC ACID
	2-Butendioic acid, dimethyl ester, (Z)-
	2-Butenedioic acid (2Z)-, 1,4-dimethyl ester
	2-Butenedioic acid (2Z)-, dimethyl ester
	2-Butenedioic acid, dimethyl ester, (Z)-
	DIMETHYL MALEATE
	Dimethyl (2Z)-but-2-enedioate
	Dimethyl cis-butenedioate
	Dimethyl cis-ethylenedicarboxylate
	Dimethylester kyseliny maleinove
	Maleic acid, dimethyl ester
	Methyl maleate
	Sipomer DMM
	cis-butenedioic acid, dimethyl ester
Inchi:	InChI=1S/C6H8O4/c1-9-5(7)3-4-6(8)10-2/h3-4H,1-2H3/b4-3-
InchiKey:	LDCRTTXIJACKKU-ARJAWSKDSA-N
Formula:	C6H8O4
SMILES:	COC(=O)C=CC(=O)OC
Mol. weight [g/mol]:	144.13
CAS:	624-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-387.98	kJ/mol	Joback Method
hf	-539.55	kJ/mol	Joback Method
hfus	17.07	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
ie	10.30	eV	NIST Webbook
ie	10.47	eV	NIST Webbook
log10ws	0.09		Crippen Method
logp	-0.111		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	3673.09	kPa	Joback Method
rinpol	1019.20		NIST Webbook
rinpol	1019.20		NIST Webbook

rinpol	979.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	984.00		NIST Webbook
tb	477.70	K	NIST Webbook
tb	475.15	K	Determination and correlation of liquid liquid equilibria for the (water + carboxylic acid + dimethyl maleate) ternary systems at T = 298.2K
tc	689.99	K	Joback Method
tf	254.00 ± 2.00	K	NIST Webbook
tf	254.00 ± 1.50	K	NIST Webbook
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.80	J/mol×K	689.99	Joback Method
cpg	235.76	J/mol×K	558.94	Joback Method
cpg	243.80	J/mol×K	591.71	Joback Method
cpg	251.49	J/mol×K	624.47	Joback Method
cpg	258.82	J/mol×K	657.23	Joback Method
cpg	218.65	J/mol×K	493.42	Joback Method
cpg	227.37	J/mol×K	526.18	Joback Method
cpl	163.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0002234	Pa×s	493.42	Joback Method
dvisc	0.0003660	Pa×s	427.82	Joback Method
dvisc	0.0004981	Pa×s	395.02	Joback Method
dvisc	0.0007168	Pa×s	362.22	Joback Method
dvisc	0.0011092	Pa×s	329.42	Joback Method
dvisc	0.0002809	Pa×s	460.62	Joback Method
dvisc	0.0018904	Pa×s	296.62	Joback Method
hfust	14.64	kJ/mol	254.00	NIST Webbook
hfust	14.64	kJ/mol	254.00	NIST Webbook
hsubt	41.80 ± 4.20	kJ/mol	329.00	NIST Webbook
hsubt	44.40 ± 4.20	kJ/mol	332.00	NIST Webbook
hvapt	52.00	kJ/mol	403.00	NIST Webbook
hvapt	53.90	kJ/mol	398.00	NIST Webbook
sfust	58.00	J/mol×K	254.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59525e+01
Coeff. B	-5.05241e+03
Coeff. C	-3.23840e+01
Temperature range (K), min.	354.91
Temperature range (K), max.	507.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.23077e+02
Coeff. B	-1.16642e+04
Coeff. C	-1.54976e+01
Coeff. D	7.06613e-06
Temperature range (K), min.	254.15
Temperature range (K), max.	675.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1071
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624486&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1071
Determination and correlation of liquid liquid equilibria for the (water + carboxylic acid + dimethylmaleate) ternary systems at T = 298.2K:	https://www.doi.org/10.1016/j.fluid.2008.04.014
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume