Butanedioic acid, dimethyl ester

Other names:	1,4-butanedioic acid, dimethyl ester
	CH3OC(O)CH2CH2C(O)OCH3
	DBE-4
	Dimethyl butanedioate
	Dimethyl ester of succinic acid
	Dimethyl succinate
	Methyl succinate
	Succinic acid, dimethyl ester
	dimethyl 1,4-butanedioate
Inchi:	InChI=1S/C6H10O4/c1-9-5(7)3-4-6(8)10-2/h3-4H2,1-2H3
InchiKey:	MUXOBHXGJLMRAB-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	COC(=O)CCC(=O)OC
Mol. weight [g/mol]:	146.14
CAS:	106-65-0

Physical Properties

Property code	Value	Unit	Source
chs	-2959.00	kJ/mol	NIST Webbook
gf	-468.20	kJ/mol	Joback Method
hf	-656.77	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	60.90 ± 0.40	kJ/mol	NIST Webbook
hvap	61.00 ± 0.30	kJ/mol	NIST Webbook
hvap	61.70 ± 0.40	kJ/mol	NIST Webbook
hvap	62.40	kJ/mol	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.113		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3060.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
rinpol	1034.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1027.00		NIST Webbook

rinpol	1026.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1035.50		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1035.50		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	169.29		NIST Webbook
rinpol	169.29		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	994.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1558.00		NIST Webbook
tb	469.80	K	Liquid liquid equilibria of the ternary system water + acetic acid + dimethyl succinate
tb	468.40 ± 2.00	K	NIST Webbook
tb	468.50 ± 2.00	K	NIST Webbook

tb	469.10 ± 1.00	K	NIST Webbook
tb	473.20	K	NIST Webbook
tb	469.60 ± 0.50	K	NIST Webbook
tb	469.60 ± 0.50	K	NIST Webbook
tb	469.40 ± 0.80	K	NIST Webbook
tb	469.60	K	NIST Webbook
tb	469.20	K	Liquid-Liquid Equilibria for Ternary Systems of Water + Formic Acid + Dibasic Esters
tc	677.07	K	Joback Method
tf	291.90 ± 0.60	K	NIST Webbook
tf	291.40 ± 1.00	K	NIST Webbook
tf	291.50 ± 0.60	K	NIST Webbook
tf	293.00 ± 1.50	K	NIST Webbook
tf	291.70 ± 2.00	K	NIST Webbook
tf	291.20 ± 2.00	K	NIST Webbook
tf	291.70 ± 2.00	K	NIST Webbook
tf	291.40 ± 1.00	K	NIST Webbook
tf	290.00 ± 1.00	K	NIST Webbook
tf	291.40 ± 1.50	K	NIST Webbook
tf	292.65 ± 0.50	K	NIST Webbook
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.42	J/mol×K	489.26	Joback Method
cpg	254.67	J/mol×K	551.86	Joback Method
cpg	287.43	J/mol×K	677.07	Joback Method
cpg	263.35	J/mol×K	583.16	Joback Method
cpg	271.71	J/mol×K	614.46	Joback Method
cpg	279.74	J/mol×K	645.76	Joback Method
cpg	245.69	J/mol×K	520.56	Joback Method
dvisc	0.0003335	Pa×s	458.00	Joback Method
dvisc	0.0004316	Pa×s	426.74	Joback Method
dvisc	0.0005818	Pa×s	395.48	Joback Method
dvisc	0.0008254	Pa×s	364.22	Joback Method
dvisc	0.0012506	Pa×s	332.96	Joback Method
dvisc	0.0002663	Pa×s	489.26	Joback Method
dvisc	0.0020653	Pa×s	301.70	Joback Method
hvapt	49.30	kJ/mol	405.00	NIST Webbook

pvap	8.30	kPa	393.49	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa
pvap	5.20	kPa	382.13	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa
pvap	2.00	kPa	363.39	Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2, 5.2 and 8.3 kPa
rfi	1.41969		293.15	(Liquid + liquid) equilibria of (water + butyric acid + dibasic esters) ternary systems
rfi	1.41969		293.15	Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems
rfi	1.41969		293.15	(Liquid + liquid) equilibria of (water + propionic acid + dibasic esters) ternary systems

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65135e+01
Coeff. B	-5.37480e+03
Coeff. C	-1.75020e+01
Temperature range (K), min.	348.75
Temperature range (K), max.	497.31

Sources

(Liquid + liquid) equilibria of (water + butyric acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2006.07.002
Liquid-Liquid Equilibria for Ternary Systems of Water + Formic Acid + Dibasic Esters:	https://www.doi.org/10.1021/je700206y
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid liquid equilibria of the ternary system water + acetic acid + dimethyl succinate:	https://www.doi.org/10.1016/j.fluid.2005.09.013
Phase equilibria of (water + levulinic acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.fluid.2009.04.017
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106650&Units=SI
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
Isobaric vapor-liquid equilibrium of three binary systems containing dimethyl succinate, dimethyl glutarate and dimethyl adipate at 2.5, 5.2 and 8.3 kPa:	https://www.doi.org/10.1016/j.jct.2019.02.006
(Liquid + liquid) equilibria of (water + propionic acid + dibasic esters) ternary systems:	https://www.doi.org/10.1016/j.jct.2007.02.012
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

Legend

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
hfus:	Enthalpy of fusion 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
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume