2-Butenedioic acid (Z)-, diethyl ester

Other names:	DIETHYL ESTER MALEIC ACID
	DIETHYL MALEATE
	Diethyl (2z)-2-butenedioate
	Diethylester kyseliny maleinove
	ETHYL MALEATE
	Maleic acid, diethyl ester
Inchi:	InChI=1S/C8H12O4/c1-3-11-7(9)5-6-8(10)12-4-2/h5-6H,3-4H2,1-2H3/b6-5-
InchiKey:	IEPRKVQEAMIZSS-WAYWQWQTSA-N
Formula:	C8H12O4
SMILES:	CCOC(=O)C=CC(=O)OCC
Mol. weight [g/mol]:	172.18
CAS:	141-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-371.14	kJ/mol	Joback Method
hf	-580.83	kJ/mol	Joback Method
hfus	22.25	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.669		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	2947.28	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1077.30		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1077.30		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1081.00		NIST Webbook
tb	498.20	K	NIST Webbook
tc	730.81	K	Joback Method
tf	319.16	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.47	J/mol×K	539.18	Joback Method
cpg	314.43	J/mol×K	571.12	Joback Method
cpg	324.91	J/mol×K	603.06	Joback Method
cpg	334.94	J/mol×K	634.99	Joback Method
cpg	344.49	J/mol×K	666.93	Joback Method
cpg	353.58	J/mol×K	698.87	Joback Method
cpg	362.20	J/mol×K	730.81	Joback Method
dvisc	0.0018749	Pa×s	319.16	Joback Method
dvisc	0.0010564	Pa×s	355.83	Joback Method
dvisc	0.0006626	Pa×s	392.50	Joback Method
dvisc	0.0004501	Pa×s	429.17	Joback Method
dvisc	0.0003249	Pa×s	465.84	Joback Method
dvisc	0.0002460	Pa×s	502.51	Joback Method
dvisc	0.0001934	Pa×s	539.18	Joback Method
hvapt	55.20	kJ/mol	414.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60472e+01
Coeff. B	-5.23300e+03
Coeff. C	-4.02720e+01
Temperature range (K), min.	372.32
Temperature range (K), max.	527.71

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.30246e+01
Coeff. B	-8.80598e+03
Coeff. C	-6.67305e+00

Coeff. D	2.85276e-06
Temperature range (K), min.	264.35
Temperature range (K), max.	680.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Phase equilibria of (water + carboxylic acid + diethyl maleate) ternary liquid systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2011.01.020
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1097
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1097

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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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