Diethyl fumarate

Other names:	2-Butenedioic acid (2E)-, 1,4-diethyl ester
	2-Butenedioic acid (2E)-, diethyl ester
	2-Butenedioic acid (E)-, diethyl ester
	2-Butenedioic acid, diethyl ester, (E)-
	ANTI-PSORIATICUM
	Diethyl (2E)-2-butenedioate
	Diethyl ester of (E)-2-Butenedioic acid
	Diethylester kyseliny fumarove
	ETHYL FUMARATE
	Fumaric acid, diethyl ester
	NSC 20954
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-AATRIKPKSA-N
Formula:	C8H12O4
SMILES:	CCOC(=O)C=CC(=O)OCC
Mol. weight [g/mol]:	172.18
CAS:	623-91-6

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	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1647.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1660.00		NIST Webbook

ripol	1647.00		NIST Webbook
tb	491.70	K	NIST Webbook
tb	487.00 ± 2.00	K	NIST Webbook
tb	491.00	K	KDB
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	362.20	J/mol×K	730.81	Joback Method
cpg	353.58	J/mol×K	698.87	Joback Method
cpg	344.49	J/mol×K	666.93	Joback Method
cpg	334.94	J/mol×K	634.99	Joback Method
cpg	324.91	J/mol×K	603.06	Joback Method
cpg	314.43	J/mol×K	571.12	Joback Method
cpg	303.47	J/mol×K	539.18	Joback Method
dvisc	0.0018749	Pa×s	319.16	Joback Method
dvisc	0.0001934	Pa×s	539.18	Joback Method
dvisc	0.0002460	Pa×s	502.51	Joback Method
dvisc	0.0003249	Pa×s	465.84	Joback Method
dvisc	0.0004501	Pa×s	429.17	Joback Method
dvisc	0.0006626	Pa×s	392.50	Joback Method
dvisc	0.0010564	Pa×s	355.83	Joback Method
hvapt	53.20	kJ/mol	409.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.93571e+01
Coeff. B	-6.92373e+03
Coeff. C	-1.75617e+00
Coeff. D	9.12753e-07
Temperature range (K), min.	326.15
Temperature range (K), max.	492.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Separation of propionic acid by diethyl carbonate or diethyl malonate or diethyl fumarate and the synergistic effect of binary solvents	https://www.doi.org/10.1016/j.fluid.2010.01.018
Determination of Vapor-Liquid Equilibria of the Binary Systems of Sub-critical CO2 and Diethyl Fumarate:	https://www.doi.org/10.1021/je4010849
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1184
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid phase equilibria of (water + formic acid + diethyl carbonate or diethyl malonate or diethyl fumarate) ternary systems at 298.15K and atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2010.08.030
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623916&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1184
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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