Dimethyl fumarate

Other names:	(E)-But-2-enedioic acid dimethyl ester
	(E)-CH3OC(O)CH=CHC(O)OCH3
	2-Butenedioic acid (2E)-, 1,4-dimethyl ester
	2-Butenedioic acid (2E)-, dimethyl ester
	2-Butenedioic acid (E)-, dimethyl ester
	2-Butenedioic acid, dimethyl ester, (E)-
	Allomaleic acid dimethyl ester
	Boletic acid dimethyl ester
	DIMETHYL MALEATE
	Dimethyl trans-ethylenedicarboxylate
	Dimethylester kyseliny fumarove
	Ethylene, 1,2-bis(methoxycarbonyl)-, trans-
	Fumaric acid, dimethyl ester
	METHYL FUMARATE
	NSC 167432
	NSC 25942
	trans-1,2-Ethylenedicarboxylic acid dimethyl ester
	trans-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-ONEGZZNKSA-N
Formula:	C6H8O4
SMILES:	COC(=O)C=CC(=O)OC
Mol. weight [g/mol]:	144.13
CAS:	624-49-7

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	10.50	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	-0.111		Crippen Method
mcvol	105.980	ml/mol	McGowan Method

pc	3673.09	kPa	Joback Method
rinpol	993.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	993.00		NIST Webbook
tb	466.20	K	NIST Webbook
tb	466.40	K	KDB
tc	689.99	K	Joback Method
tf	375.00 ± 1.00	K	NIST Webbook
tf	375.00 ± 2.00	K	NIST Webbook
tf	374.70 ± 0.60	K	NIST Webbook
tf	376.65	K	Aqueous Solubility Prediction Method
tf	374.85	K	KDB
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.82	J/mol×K	657.23	Joback Method
cpg	251.49	J/mol×K	624.47	Joback Method
cpg	265.80	J/mol×K	689.99	Joback Method
cpg	218.65	J/mol×K	493.42	Joback Method
cpg	227.37	J/mol×K	526.18	Joback Method
cpg	235.76	J/mol×K	558.94	Joback Method
cpg	243.80	J/mol×K	591.71	Joback Method
cps	199.20	J/mol×K	298.00	NIST Webbook
dvisc	0.0003660	Pa×s	427.82	Joback Method
dvisc	0.0002809	Pa×s	460.62	Joback Method
dvisc	0.0002234	Pa×s	493.42	Joback Method
dvisc	0.0018904	Pa×s	296.62	Joback Method
dvisc	0.0011092	Pa×s	329.42	Joback Method
dvisc	0.0007168	Pa×s	362.22	Joback Method
dvisc	0.0004981	Pa×s	395.02	Joback Method
hfust	35.15	kJ/mol	375.00	NIST Webbook
hfust	35.15	kJ/mol	375.00	NIST Webbook
hfust	35.15	kJ/mol	375.00	NIST Webbook

hsubt	85.00 ± 2.00	kJ/mol	283.00	NIST Webbook
hvapt	53.80	kJ/mol	413.50	NIST Webbook
sfust	94.00	J/mol×K	375.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.83179e+01
Coeff. B	-6.46339e+03
Coeff. C	-1.27978e-04
Coeff. D	1.22359e-10
Temperature range (K), min.	361.15
Temperature range (K), max.	466.15

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C624497&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1174
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1174

Legend

cpg: Ideal gas heat capacity
cps: Solid 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
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