Fumaric Acid

Other names:	(E)-2-Butenedioic acid
	(E)-HO2CCH=CHCO2H
	1,2-Ethenedicarboxylic acid, trans-
	1,2-Ethylenedicarboxylic acid, (E)
	2-Butenedioic acid (2E)-
	2-Butenedioic acid (E)-
	Allomaleic acid
	Boletic acid
	Butenedioic acid, (E)-
	Kyselina fumarova
	Lichenic acid
	NSC-2752
	TRANS-1,2-ETHYLENEDICARBOXYL ACID
	TRANS-BUTENEDIOIC ACID
	Tumaric acid
	U-1149
	USAF EK-P-583
	trans-1,2-Ethylenedicarboxylic Acid
Inchi:	InChI=1S/C4H4O4/c5-3(6)1-2-4(7)8/h1-2H,(H,5,6)(H,7,8)/b2-1+
InchiKey:	VZCYOOQTPOCHFL-OWOJBTEDSA-N
Formula:	C4H4O4
SMILES:	O=C(O)C=CC(=O)O
Mol. weight [g/mol]:	116.07
CAS:	110-17-8

Physical Properties

Property code	Value	Unit	Source
chs	-1333.50	kJ/mol	NIST Webbook
chs	-1334.70	kJ/mol	NIST Webbook
chs	-1334.70 ± 0.80	kJ/mol	NIST Webbook
gf	-468.46	kJ/mol	Joback Method
hf	-538.29	kJ/mol	Joback Method
hfl	-810.20 ± 1.30	kJ/mol	NIST Webbook
hfs	-812.24	kJ/mol	NIST Webbook
hfs	-810.98	kJ/mol	NIST Webbook
hfs	-811.03 ± 0.88	kJ/mol	NIST Webbook
hfus	17.69	kJ/mol	Joback Method

hvap	71.31	kJ/mol	Joback Method
ie	10.90	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	0.45		Crippen Method
logp	-0.288		Crippen Method
mcvol	77.800	ml/mol	McGowan Method
pc	6503.64	kPa	Joback Method
ss	166.10	J/mol×K	NIST Webbook
tb	587.18	K	Joback Method
tc	769.82	K	Joback Method
tf	560.45 ± 4.00	K	NIST Webbook
tf	557.15 ± 4.00	K	NIST Webbook
tf	473.00 ± 4.00	K	NIST Webbook
tf	375.00 ± 2.00	K	NIST Webbook
tf	562.55 ± 0.50	K	NIST Webbook
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.74	J/mol×K	739.38	Joback Method
cpg	180.57	J/mol×K	678.50	Joback Method
cpg	176.64	J/mol×K	648.06	Joback Method
cpg	172.46	J/mol×K	617.62	Joback Method
cpg	168.01	J/mol×K	587.18	Joback Method
cpg	184.27	J/mol×K	708.94	Joback Method
cpg	191.01	J/mol×K	769.82	Joback Method
cps	141.80	J/mol×K	297.10	NIST Webbook
dvisc	0.0094225	Pa×s	351.26	Joback Method
dvisc	0.0000492	Pa×s	587.18	Joback Method
dvisc	0.0000862	Pa×s	547.86	Joback Method
dvisc	0.0001649	Pa×s	508.54	Joback Method
dvisc	0.0003515	Pa×s	469.22	Joback Method
dvisc	0.0008609	Pa×s	429.90	Joback Method
dvisc	0.0025249	Pa×s	390.58	Joback Method
hsubt	134.00 ± 4.20	kJ/mol	364.50	NIST Webbook
hsubt	136.00 ± 6.30	kJ/mol	365.00	NIST Webbook
hsubt	123.60 ± 2.00	kJ/mol	381.00	NIST Webbook
hsubt	136.00 ± 6.30	kJ/mol	365.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.38448e+02
Coeff. B	-2.24627e+04
Coeff. C	-3.11521e+01
Coeff. D	1.05833e-05
Temperature range (K), min.	560.15
Temperature range (K), max.	771.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=961
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=961
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110178&Units=SI

Legend

chs: Standard solid enthalpy of combustion
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
hfl: Liquid phase enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume