2-Butenoic acid, (E)-

Other names:	(E)-2-BUTENOIC ACID
	(E)-CH3CH=CHCOOH
	(E)-CROTONIC ACID
	2-Butenoic acid, (2E)-
	3-Methylacrylic acid, trans
	Crotonic acid
	Crotonic acid, (E)-
	Crotonic acid, trans
	Ethylideneacetic acid, E
	NSC 8751
	TRANS-CROTONIC ACID
	trans-2-Butenoic Acid
	«alpha»-butenoic acid, trans
	«alpha»-crotonic acid, trans
	«beta»-Methacrylic acid, trans
	«beta»-methylacrylic acid, trans
	Â«alphaÂ»-butenoic acid, trans
	Â«alphaÂ»-crotonic acid, trans
	Â«betaÂ»-Methacrylic acid, trans
	Â«betaÂ»-methylacrylic acid, trans
Inchi:	InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/b3-2+
InchiKey:	LDHQCZJRKDOVOX-NSCUHMNNSA-N
Formula:	C4H6O2
SMILES:	CC=CC(=O)O
Mol. weight [g/mol]:	86.09
CAS:	107-93-7

Physical Properties

Property code	Value	Unit	Source
affp	824.00	kJ/mol	NIST Webbook
basg	793.00	kJ/mol	NIST Webbook
chl	-2000.00	kJ/mol	NIST Webbook
chl	-2085.00	kJ/mol	NIST Webbook
gf	-202.72	kJ/mol	Joback Method
hf	-273.48	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method

ie	10.28	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	9.90 ± 0.10	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-0.45		Crippen Method
logp	0.647		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
ripol	1740.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1740.00		NIST Webbook
tb	453.70	K	NIST Webbook
tb	458.20	K	NIST Webbook
tc	623.44	K	Joback Method
tf	344.70 ± 1.00	K	NIST Webbook
tf	344.80 ± 0.60	K	NIST Webbook
tf	344.60 ± 0.40	K	NIST Webbook
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.47	J/mol×K	441.13	Joback Method
cpg	135.50	J/mol×K	471.51	Joback Method
cpg	141.22	J/mol×K	501.90	Joback Method
cpg	146.65	J/mol×K	532.28	Joback Method
cpg	151.79	J/mol×K	562.67	Joback Method
cpg	156.65	J/mol×K	593.05	Joback Method
cpg	161.26	J/mol×K	623.44	Joback Method
dvisc	0.0325411	Pa×s	240.51	Joback Method
dvisc	0.0085700	Pa×s	273.95	Joback Method
dvisc	0.0030171	Pa×s	307.38	Joback Method
dvisc	0.0013037	Pa×s	340.82	Joback Method
dvisc	0.0006544	Pa×s	374.26	Joback Method
dvisc	0.0003678	Pa×s	407.69	Joback Method
dvisc	0.0002256	Pa×s	441.13	Joback Method
hvapt	56.70	kJ/mol	405.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57176e+01
Coeff. B	-4.03838e+03
Coeff. C	-8.98580e+01
Temperature range (K), min.	344.55
Temperature range (K), max.	483.83

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.03769e+02
Coeff. B	-1.09030e+04
Coeff. C	-1.24614e+01
Coeff. D	4.65069e-06
Temperature range (K), min.	344.55
Temperature range (K), max.	666.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=975

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=975

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107937&Units=SI

Legend

affp: Proton affinity

basg:	Gas basicity
chl:	Standard liquid 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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume