2-Butenoic acid, methyl ester, (E)-

Other names:	(E)-2-Butenoic acid methyl ester
	(E)-CH3CH=CHC(O)OCH3
	(E)-Crotonic acid methyl ester
	2-Butenoic acid, methyl ester, (2E)-
	Crotonic acid, methyl ester, (E)-
	Methyl (E)-2-butenoate
	Methyl 2-butenoate, (E)-
	Methyl E-crotonate
	Methyl E-propene-1-carboxylate
	Methyl crotonate
	Methyl crotonate, (E)-
	Methyl trans-2-butenoate
	Methyl trans-crotonate
	Methyl «alpha»-crotonate, trans-
	Methyl Â«alphaÂ»-crotonate, trans-
	trans-2-Butenoic acid methyl ester
Inchi:	InChI=1S/C5H8O2/c1-3-4-5(6)7-2/h3-4H,1-2H3/b4-3+
InchiKey:	MCVVUJPXSBQTRZ-ONEGZZNKSA-N
Formula:	C5H8O2
SMILES:	CC=CC(=O)OC
Mol. weight [g/mol]:	100.12
CAS:	623-43-8

Physical Properties

Property code	Value	Unit	Source
affp	851.30	kJ/mol	NIST Webbook
basg	820.40	kJ/mol	NIST Webbook
chl	-2728.00	kJ/mol	NIST Webbook
gf	-162.48	kJ/mol	Joback Method
hf	-342.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-383.00 ± 2.00	kJ/mol	NIST Webbook
hfus	11.69	kJ/mol	Joback Method
hvap	41.00 ± 1.00	kJ/mol	NIST Webbook
hvap	41.00	kJ/mol	NIST Webbook
log10ws	-0.63		Crippen Method
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method

pc	3906.25	kPa	Joback Method
rinpol	753.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	745.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1088.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	394.20	K	NIST Webbook
tb	392.20	K	NIST Webbook
tc	582.22	K	Joback Method
tf	213.19	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.24	J/mol×K	394.25	Joback Method
cpg	185.52	J/mol×K	550.89	Joback Method
cpg	178.67	J/mol×K	519.56	Joback Method
cpg	171.53	J/mol×K	488.23	Joback Method
cpg	164.08	J/mol×K	456.91	Joback Method
cpg	156.32	J/mol×K	425.58	Joback Method
cpg	192.07	J/mol×K	582.22	Joback Method
dvisc	0.0002253	Pa×s	394.25	Joback Method
dvisc	0.0002854	Pa×s	364.07	Joback Method
dvisc	0.0003774	Pa×s	333.90	Joback Method
dvisc	0.0005276	Pa×s	303.72	Joback Method

dvisc	0.0007942	Pa×s	273.54	Joback Method
dvisc	0.0013230	Pa×s	243.37	Joback Method
dvisc	0.0025463	Pa×s	213.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56634e+01
Coeff. B	-3.77162e+03
Coeff. C	-5.07240e+01
Temperature range (K), min.	296.02
Temperature range (K), max.	415.06

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623438&Units=SI

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

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

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

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

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume