

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

<b>Other names:</b>	(E)-2-Butenoic acid methyl ester (E)-CH <sub>3</sub> CH=CHC(O)OCH <sub>3</sub> (E)-Crotonic acid methyl ester 2-Butenoic acid, methyl ester, (2E)- Crotonic acid, methyl ester, (E)- Methyl (E)-2-butenolate Methyl 2-butenolate, (E)- Methyl E-crotonate Methyl E-propene-1-carboxylate Methyl crotonate Methyl crotonate, (E)- Methyl trans-2-butenolate Methyl trans-crotonate Methyl «alpha»-crotonate, trans- Methyl «alpha»-crotonate, trans- trans-2-Butenoic acid methyl ester
<b>Inchi:</b>	InChI=1S/C5H8O2/c1-3-4-5(6)7-2/h3-4H,1-2H3/b4-3+
<b>InchiKey:</b>	MCVVUJXPXSBQTRZ-ONEGZZNKSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>
<b>SMILES:</b>	CC=CC(=O)OC
<b>Mol. weight [g/mol]:</b>	100.12
<b>CAS:</b>	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	kJ/mol	NIST Webbook
hvap	41.00 ± 1.00	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	761.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	756.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1088.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	392.20	K	NIST Webbook
tb	394.20	K	NIST Webbook
tc	582.22	K	Joback Method
tf	213.19	K	Joback Method
vc	0.320	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

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

dvisc	0.0007942	Paxs	273.54	Joback Method
dvisc	0.0013230	Paxs	243.37	Joback Method
dvisc	0.0025463	Paxs	213.19	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C623438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C623438&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions

<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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