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

Other names:	Crotonic acid, ethyl ester, (E)-
	trans-2-Butenoic acid ethyl ester
	Ethyl (E)-crotonate
	Ethyl trans-crotonate
	(E)-2-Butenoic acid ethyl ester
	(E)-CH3CH=CHCOOC2H5
	Crotonate d'ethyle, E-
	«alpha»-Crotonic acid ethyl ester, trans-
	Ethyl (E)-2-butenoate
	Ethyl trans-2-butenoate
	2-Butenoic acid, ethyl ester, (2E)-
	Ethyl crotonate
Inchi:	InChI=1S/C6H10O2/c1-3-5-6(7)8-4-2/h3,5H,4H2,1-2H3/b5-3+
InchiKey:	ZFDIRQKJPRINOQ-HWKANZROSA-N
Formula:	C6H10O2
SMILES:	CC=CC(=O)OCC
Mol. weight [g/mol]:	114.14
CAS:	623-70-1

Physical Properties

Property code	Value	Unit	Source
chl	-3370.20 ± 2.10	kJ/mol	NIST Webbook
gf	-154.06	kJ/mol	Joback Method
hf	-376.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-420.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.28	kJ/mol	Joback Method
hvap	44.00	kJ/mol	NIST Webbook
hvap	44.00 ± 1.00	kJ/mol	NIST Webbook
ie	10.11	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	834.00		NIST Webbook

rinpol	812.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	844.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	844.00	NIST Webbook
rinpol	851.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	848.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	830.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1164.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1151.00	NIST Webbook
ripol	1158.00	NIST Webbook
ripol	1157.00	NIST Webbook
ripol	1167.00	NIST Webbook
ripol	1169.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1157.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1153.00	NIST Webbook
ripol	1161.00	NIST Webbook
ripol	1153.00	NIST Webbook
ripol	1158.00	NIST Webbook

tb	415.70	K	NIST Webbook
tb	409.70	K	NIST Webbook
tc	599.00 ± 5.00	K	NIST Webbook
tf	224.46	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.29	J/mol×K	417.13	Joback Method
cpg	193.78	J/mol×K	448.23	Joback Method
cpg	202.88	J/mol×K	479.33	Joback Method
cpg	211.61	J/mol×K	510.43	Joback Method
cpg	219.98	J/mol×K	541.53	Joback Method
cpg	227.98	J/mol×K	572.63	Joback Method
cpg	235.63	J/mol×K	603.73	Joback Method
dvisc	0.0027763	Pa×s	224.46	Joback Method
dvisc	0.0014062	Pa×s	256.57	Joback Method
dvisc	0.0008286	Pa×s	288.68	Joback Method
dvisc	0.0005428	Pa×s	320.80	Joback Method
dvisc	0.0003840	Pa×s	352.91	Joback Method
dvisc	0.0002879	Pa×s	385.02	Joback Method
dvisc	0.0002255	Pa×s	417.13	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623701&Units=SI

Legend

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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