Ethyl 2-butenoate

Other names:	2-Butenoic acid, ethyl ester
	ethyl but-2-enoate
	ethyl crotonate
Inchi:	InChI=1S/C6H10O2/c1-3-5-6(7)8-4-2/h3,5H,4H2,1-2H3
InchiKey:	ZFDIRQKJPRINOQ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC=CC(=O)OCC
Mol. weight [g/mol]:	114.14
CAS:	10544-63-5

Physical Properties

Property code	Value	Unit	Source
gf	-154.06	kJ/mol	Joback Method
hf	-294.75	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	826.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1169.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1149.00		NIST Webbook

ripol	1165.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1146.00		NIST Webbook
ripol	1122.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1179.90		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1122.00		NIST Webbook
tb	417.13	K	Joback Method
tc	603.73	K	Joback Method
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
hvapt	47.10	kJ/mol	374.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70693e+01
Coeff. B	-4.25541e+03
Coeff. C	-5.50330e+01
Temperature range (K), min.	308.61
Temperature range (K), max.	416.95

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10544635&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

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
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