ethyl trans-2-butenoate

Other names:	crotonic acid, ethyl ester
	ethyl crotonate
	trans-2-butenoic acid, ethyl ester
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
af	0.3965		Cheméo Relay (1.0)
gf	-154.06	kJ/mol	Joback Method
hf	-376.59	kJ/mol	Cheméo Relay (1.0)
hfus	14.28	kJ/mol	Joback Method
hvap	42.60	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-1.54		Cheméo Relay (1.0)
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3670.80	kPa	Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements
tb	403.04	K	Cheméo Relay (1.0)
tc	586.93	K	Cheméo Relay (1.0)
tf	220.39	K	Cheméo Relay (1.0)
vc	0.356	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49916e+01
Coeff. B	-3.73696e+03
Coeff. C	-5.54500e+01
Temperature range (K), min.	309.60
Temperature range (K), max.	441.50

Sources

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

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

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

Cheméo Relay (1.0, beta):

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements: https://www.doi.org/10.1021/je5002494

Legend

af:	Acentric Factor
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume