3-Butenoic acid, ethyl ester

Other names:	Ethyl 3-butenoate
Inchi:	InChI=1S/C6H10O2/c1-3-5-6(7)8-4-2/h3H,1,4-5H2,2H3
InchiKey:	BFMKFCLXZSUVPI-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=CCC(=O)OCC
Mol. weight [g/mol]:	114.14
CAS:	1617-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-146.44	kJ/mol	Joback Method
hf	-286.54	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	767.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	770.00		NIST Webbook
ripol	1105.00		NIST Webbook
tb	409.65	K	Joback Method
tc	590.97	K	Joback Method
tf	227.78	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.90	J/mol×K	409.65	Joback Method
cpg	227.57	J/mol×K	560.75	Joback Method
cpg	219.68	J/mol×K	530.53	Joback Method
cpg	211.47	J/mol×K	500.31	Joback Method

cpg	202.94	J/mol×K	470.09	Joback Method
cpg	194.08	J/mol×K	439.87	Joback Method
cpg	235.15	J/mol×K	590.97	Joback Method
dvisc	0.0002688	Pa×s	409.65	Joback Method
dvisc	0.0003382	Pa×s	379.34	Joback Method
dvisc	0.0004430	Pa×s	349.03	Joback Method
dvisc	0.0006108	Pa×s	318.72	Joback Method
dvisc	0.0009008	Pa×s	288.40	Joback Method
dvisc	0.0014557	Pa×s	258.09	Joback Method
dvisc	0.0026729	Pa×s	227.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48589e+01
Coeff. B	-3.54977e+03
Coeff. C	-5.01680e+01
Temperature range (K), min.	293.78
Temperature range (K), max.	421.97

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1617181&Units=SI

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
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

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