

3-Butenoic acid, ethyl ester

Other names:	Ethyl 3-butenolate
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	770.00		NIST Webbook
rinpol	767.00		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/molxK	409.65	Joback Method
cpg	194.08	J/molxK	439.87	Joback Method
cpg	202.94	J/molxK	470.09	Joback Method
cpg	211.47	J/molxK	500.31	Joback Method

cpg	219.68	J/molxK	530.53	Joback Method
cpg	227.57	J/molxK	560.75	Joback Method
cpg	235.15	J/molxK	590.97	Joback Method
dvisc	0.0026729	Paxs	227.78	Joback Method
dvisc	0.0014557	Paxs	258.09	Joback Method
dvisc	0.0009008	Paxs	288.40	Joback Method
dvisc	0.0006108	Paxs	318.72	Joback Method
dvisc	0.0004430	Paxs	349.03	Joback Method
dvisc	0.0003382	Paxs	379.34	Joback Method
dvisc	0.0002688	Paxs	409.65	Joback Method

Correlations

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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