Butanoic acid, ethenyl ester

Other names:	Butyric acid, vinyl ester
	UN 2838
	Vinyl butanoate
	Vinyl butyrate, inhibited
	Vinylester kyseliny maselne
	n-Butyric acid vinyl ester
Inchi:	InChI=1S/C6H10O2/c1-3-5-6(7)8-4-2/h4H,2-3,5H2,1H3
InchiKey:	MEGHWIAOTJPCHQ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=COC(=O)CCC
Mol. weight [g/mol]:	114.14
CAS:	123-20-6

Physical Properties

Property code	Value	Unit	Source
af	0.4818		Cheméo Relay (1.0)
hf	-362.72	kJ/mol	Cheméo Relay (1.0)
hfus	12.80	kJ/mol	Joback Method
hvap	37.54	kJ/mol	Cheméo Relay (1.0)
ie	9.29	eV	Cheméo Relay (1.0)
log10ws	-1.23		Cheméo Relay (1.0)
logp	1.473		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	750.00		NIST Webbook
ripol	1045.00		NIST Webbook
ripol	1045.00		NIST Webbook
ripol	1045.00		NIST Webbook

tb	389.00	K	NIST Webbook
tc	560.93	K	Cheméo Relay (1.0)
tf	178.99	K	Cheméo Relay (1.0)
vc	0.358	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.15	J/mol×K	590.97	Joback Method
cpg	219.68	J/mol×K	530.53	Joback Method
cpg	184.90	J/mol×K	409.65	Joback Method
cpg	194.08	J/mol×K	439.87	Joback Method
cpg	202.94	J/mol×K	470.09	Joback Method
cpg	211.47	J/mol×K	500.31	Joback Method
cpg	227.57	J/mol×K	560.75	Joback Method
dvisc	0.0026729	Pa×s	227.78	Joback Method
dvisc	0.0014557	Pa×s	258.09	Joback Method
dvisc	0.0009008	Pa×s	288.40	Joback Method
dvisc	0.0006108	Pa×s	318.72	Joback Method
dvisc	0.0004430	Pa×s	349.03	Joback Method
dvisc	0.0003382	Pa×s	379.34	Joback Method
dvisc	0.0002688	Pa×s	409.65	Joback Method
hvapt	39.30	kJ/mol	376.00	NIST Webbook
rfi	1.40494		303.15	Liquid-liquid equilibria for ternary mixtures of 1-alkyl-3-methyl imidazolium bis{(trifluoromethyl)sulfonyl}imides, n-hexane and organic compounds at 303.15 K and 0.1 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55567e+01

Coeff. B	-3.71325e+03
Coeff. C	-4.95280e+01
Temperature range (K), min.	292.72
Temperature range (K), max.	411.97

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Liquid-liquid equilibria for ternary mixtures of 1-alkyl-3-methyl imidazolium bis{(trifluoromethyl)sulfonyl}imides, n-hexane and organic compounds at 298.15 K and 0.1 MPa:	https://www.doi.org/10.1016/j.jct.2016.08.033
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123206&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
rfi:	Refractive Index
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