3-Butenoic acid

Other names:	Acetic acid, ethenyl-
	CH2=CHCH2COOH
	Vinylacetic acid
	but-3-enoic acid
	«beta»-Butenoic acid
	Â«betaÂ»-Butenoic acid
Inchi:	InChI=1S/C4H6O2/c1-2-3-4(5)6/h2H,1,3H2,(H,5,6)
InchiKey:	PVEOYINWKBTPIZ-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	C=CCC(=O)O
Mol. weight [g/mol]:	86.09
CAS:	625-38-7

Physical Properties

Property code	Value	Unit	Source
gf	-195.10	kJ/mol	Joback Method
hf	-265.27	kJ/mol	Joback Method
hfus	10.52	kJ/mol	Joback Method
hvap	47.25	kJ/mol	Joback Method
ie	10.02	eV	NIST Webbook
ie	9.75	eV	NIST Webbook
log10ws	-0.45		Crippen Method
logp	0.647		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	4703.44 ± 100.00	kPa	NIST Webbook
ripol	1627.00		NIST Webbook
tb	436.20	K	NIST Webbook
tc	644.60 ± 3.00	K	NIST Webbook
tf	243.83	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	130.77	J/mol×K	433.65	Joback Method
cpg	136.62	J/mol×K	463.22	Joback Method
cpg	142.21	J/mol×K	492.78	Joback Method
cpg	147.53	J/mol×K	522.35	Joback Method
cpg	152.61	J/mol×K	551.92	Joback Method
cpg	157.44	J/mol×K	581.48	Joback Method
cpg	162.04	J/mol×K	611.05	Joback Method
dvisc	0.0295733	Pa×s	243.83	Joback Method
dvisc	0.0087410	Pa×s	275.47	Joback Method
dvisc	0.0033211	Pa×s	307.10	Joback Method
dvisc	0.0015119	Pa×s	338.74	Joback Method
dvisc	0.0007873	Pa×s	370.38	Joback Method
dvisc	0.0004543	Pa×s	402.01	Joback Method
dvisc	0.0002841	Pa×s	433.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37511e+01
Coeff. B	-2.95386e+03
Coeff. C	-1.19426e+02
Temperature range (K), min.	338.82
Temperature range (K), max.	469.43

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=C625387&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume