3-Butenoic acid, 2,2-dimethyl-

Other names: 2,2-Dimethyl-3-butenoic acid
CH2=CHC(CH3)2COOH
Inchi: InChI=1S/C6H10O2/c1-4-6(2,3)5(7)8/h4H,1H2,2-3H3,(H,7,8)
InchiKey: SCFWAOWWAANBPY-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: C=CC(C)(C)C(=O)O
Mol. weight [g/mol]: 114.14
CAS: 10276-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-175.42	kJ/mol	Joback Method
hf	-315.30	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.283		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	458.20	K	NIST Webbook
tc	661.45	K	Joback Method
tf	268.79	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.92	J/mol×K	476.18	Joback Method
cpg	250.25	J/mol×K	630.58	Joback Method
cpg	243.15	J/mol×K	599.70	Joback Method
cpg	235.59	J/mol×K	568.82	Joback Method
cpg	227.55	J/mol×K	537.94	Joback Method
cpg	219.00	J/mol×K	507.06	Joback Method
cpg	256.93	J/mol×K	661.45	Joback Method

dvisc	0.0002142	Pa×s	476.18	Joback Method
dvisc	0.0003517	Pa×s	441.62	Joback Method
dvisc	0.0006281	Pa×s	407.05	Joback Method
dvisc	0.0012494	Pa×s	372.49	Joback Method
dvisc	0.0028607	Pa×s	337.92	Joback Method
dvisc	0.0079106	Pa×s	303.36	Joback Method
dvisc	0.0284161	Pa×s	268.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	3.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56743e+01
Coeff. B	-4.30836e+03
Coeff. C	-6.85160e+01
Temperature range (K), min.	348.52
Temperature range (K), max.	484.27

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10276092&Units=SI

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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume