2-Butenoic acid, 3-methyl-

Other names:	(CH3)2C=CHCOOH
	3,3-Dimethylacrylic acid
	3-Methyl-2-butenoic acid
	3-Methylbut-2-enoic acid
	3-Methylcrotonic acid
	3-methyl-buten-2-oic-acid
	Crotonic acid, 3-methyl-
	Kyselina 3-methyl-2-butenova
	NSC 2549
	Senecic acid
	Senecioic acid
	«beta»,«beta»-Dimethacrylic acid
	«beta»,«beta»-Dimethylacrylic acid
	«beta»-Methylcrotonic acid
	Â«betaÂ»,Â«betaÂ»-Dimethacrylic acid
	Â«betaÂ»,Â«betaÂ»-Dimethylacrylic acid
	Â«betaÂ»-Methylcrotonic acid
Inchi:	InChI=1S/C5H8O2/c1-4(2)3-5(6)7/h3H,1-2H3,(H,6,7)
InchiKey:	YYPNJNDODFVZLE-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC(C)=CC(=O)O
Mol. weight [g/mol]:	100.12
CAS:	541-47-9

Physical Properties

Property code	Value	Unit	Source
affp	822.90	kJ/mol	NIST Webbook
basg	791.90	kJ/mol	NIST Webbook
gf	-202.85	kJ/mol	Joback Method
hf	-303.91	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
ie	9.63	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	3609.92 ± 95.00	kPa	NIST Webbook

rinpol	953.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	467.70	K	NIST Webbook
tc	661.84 ± 3.00	K	NIST Webbook
tf	339.15	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.62	J/mol×K	463.89	Joback Method
cpg	174.00	J/mol×K	494.57	Joback Method
cpg	181.01	J/mol×K	525.24	Joback Method
cpg	187.67	J/mol×K	555.92	Joback Method
cpg	193.97	J/mol×K	586.60	Joback Method
cpg	199.96	J/mol×K	617.27	Joback Method
cpg	205.63	J/mol×K	647.95	Joback Method
hvapt	57.70	kJ/mol	418.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35120e+01
Coeff. B	-2.88724e+03
Coeff. C	-1.43060e+02

Temperature range (K), min.	343.15
Temperature range (K), max.	495.14

Sources

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=C541479&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
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
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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