2-Butenoic acid, 3-methyl-, methyl ester

Other names:	3-Methyl-2-butenoic acid, methyl ester
	3-Methylcrotonic acid methyl ester
	Crotonic acid, 3-methyl-, methyl ester
	Methyl 3,3-dimethacrylate
	Methyl 3,3-dimethylacrylate
	Methyl 3-methyl-2-butenoate
	Methyl 3-methylbut-2-enoate
	Methyl 3-methylcrotonate
	Methyl senecioate
	Methyl «beta»-methylcrotonate
	Methyl Â«betaÂ»-methylcrotonate
Inchi:	InChI=1S/C6H10O2/c1-5(2)4-6(7)8-3/h4H,1-3H3
InchiKey:	FZIBCCGGICGWBP-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	COC(=O)C=C(C)C
Mol. weight [g/mol]:	114.14
CAS:	924-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-162.61	kJ/mol	Joback Method
hf	-304.54	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	46.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	842.40		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	833.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1184.00		NIST Webbook

ripol	1155.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1180.00		NIST Webbook
tb	417.01	K	Joback Method
tc	607.33	K	Joback Method
tf	210.50	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.26	J/mol×K	417.01	Joback Method
cpg	193.90	J/mol×K	448.73	Joback Method
cpg	203.14	J/mol×K	480.45	Joback Method
cpg	212.00	J/mol×K	512.17	Joback Method
cpg	220.47	J/mol×K	543.89	Joback Method
cpg	228.57	J/mol×K	575.61	Joback Method
cpg	236.31	J/mol×K	607.33	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70693e+01
Coeff. B	-4.25541e+03
Coeff. C	-5.50330e+01
Temperature range (K), min.	308.61
Temperature range (K), max.	416.95

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=C924505&Units=SI

Legend

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
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