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

Other names:	3,3-Dimethylacrylic acid ethyl ester
	3-Methyl-2-butenoic acid, ethyl ester
	Crotonic acid, 3-methyl-, ethyl ester
	Ethyl 3,3-dimethylacrylate
	Ethyl 3-methyl-2-butenoate
	Ethyl 3-methylbut-2-enoate
	Ethyl 3-methylcrotonate
	Ethyl dimethylacrylate
	Ethyl isobutenoate
	Ethyl isopropylideneacetate
	Ethyl senecioate
	Ethyl «beta»,«beta»-dimethylacrylate
	Ethyl «beta»-methylcrotonate
	Ethyl Â«betaÂ»,Â«betaÂ»-dimethylacrylate
	Ethyl Â«betaÂ»-methylcrotonate
	NSC 61853
	NSC 99208
Inchi:	InChI=1S/C7H12O2/c1-4-9-7(8)5-6(2)3/h5H,4H2,1-3H3
InchiKey:	UTXVCHVLDOLVPC-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCOC(=O)C=C(C)C
Mol. weight [g/mol]:	128.17
CAS:	638-10-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	49.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	911.00		NIST Webbook

rinpol	911.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	911.00		NIST Webbook
ripol	1217.00		NIST Webbook
ripol	1219.00		NIST Webbook
tb	426.70	K	NIST Webbook
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/mol×K	439.89	Joback Method
cpg	233.55	J/mol×K	471.32	Joback Method
cpg	244.02	J/mol×K	502.76	Joback Method
cpg	254.05	J/mol×K	534.19	Joback Method
cpg	263.64	J/mol×K	565.63	Joback Method
cpg	272.80	J/mol×K	597.06	Joback Method
cpg	281.54	J/mol×K	628.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61219e+01
Coeff. B	-4.15272e+03
Coeff. C	-5.97590e+01
Temperature range (K), min.	322.02
Temperature range (K), max.	443.90

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638108&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
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

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