Methyl 3-butenoate

Other names:	3-Butenoic acid, methyl ester
	CH2=CHCH2C(O)OCH3
Inchi:	InChI=1S/C5H8O2/c1-3-4-5(6)7-2/h3H,1,4H2,2H3
InchiKey:	GITITJADGZYSRL-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	C=CCC(=O)OC
Mol. weight [g/mol]:	100.12
CAS:	3724-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.86	kJ/mol	Joback Method
hf	-265.90	kJ/mol	Joback Method
hfus	10.21	kJ/mol	Joback Method
hvap	35.21	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	718.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	692.00		NIST Webbook
tb	386.77	K	Joback Method
tc	569.17	K	Joback Method
tf	216.51	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.35	J/mol×K	386.77	Joback Method
cpg	157.10	J/mol×K	417.17	Joback Method

cpg	164.59	J/mol×K	447.57	Joback Method
cpg	171.82	J/mol×K	477.97	Joback Method
cpg	178.80	J/mol×K	508.37	Joback Method
cpg	185.52	J/mol×K	538.77	Joback Method
cpg	191.98	J/mol×K	569.17	Joback Method
dvisc	0.0024241	Pa×s	216.51	Joback Method
dvisc	0.0013568	Pa×s	244.89	Joback Method
dvisc	0.0008567	Pa×s	273.26	Joback Method
dvisc	0.0005898	Pa×s	301.64	Joback Method
dvisc	0.0004330	Pa×s	330.02	Joback Method
dvisc	0.0003338	Pa×s	358.39	Joback Method
dvisc	0.0002673	Pa×s	386.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73439e+01
Coeff. B	-4.10370e+03
Coeff. C	-4.82220e+01
Temperature range (K), min.	288.82
Temperature range (K), max.	389.28

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=C3724558&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume