2-Butenoic acid, methyl ester, (Z)-

Other names: Crotonic acid, methyl ester, (Z)-
Methyl (Z)-2-butenoate
Methyl cis-2-butenoate
Inchi: InChI=1S/C5H8O2/c1-3-4-5(6)7-2/h3-4H,1-2H3/b4-3-
InchiKey: MCVVUJPXSBQTRZ-ARJAWSKDSA-N
Formula: C5H8O2
SMILES: CC=CC(=O)OC
Mol. weight [g/mol]: 100.12
CAS: 4358-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-162.48	kJ/mol	Joback Method
hf	-274.11	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	35.84	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	726.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	726.00		NIST Webbook
ripol	1032.00		NIST Webbook
ripol	1032.00		NIST Webbook
tb	394.25	K	Joback Method
tc	582.22	K	Joback Method
tf	213.19	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.24	J/mol×K	394.25	Joback Method

cpg	156.32	J/mol×K	425.58	Joback Method
cpg	164.08	J/mol×K	456.91	Joback Method
cpg	171.53	J/mol×K	488.23	Joback Method
cpg	178.67	J/mol×K	519.56	Joback Method
cpg	185.52	J/mol×K	550.89	Joback Method
cpg	192.07	J/mol×K	582.22	Joback Method
dvisc	0.0025463	Pa×s	213.19	Joback Method
dvisc	0.0013230	Pa×s	243.37	Joback Method
dvisc	0.0007942	Pa×s	273.54	Joback Method
dvisc	0.0005276	Pa×s	303.72	Joback Method
dvisc	0.0003774	Pa×s	333.90	Joback Method
dvisc	0.0002854	Pa×s	364.07	Joback Method
dvisc	0.0002253	Pa×s	394.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83123e+01
Coeff. B	-4.39316e+03
Coeff. C	-4.98900e+01
Temperature range (K), min.	293.62
Temperature range (K), max.	387.80

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=C4358592&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume