2-Butenoic acid, methyl ester

Other names:	Crotonic acid, methyl ester
	Methyl crotonate
	Methyl 2-butenoate
	Methyl but-2-enoate
Inchi:	InChI=1S/C5H8O2/c1-3-4-5(6)7-2/h3-4H,1-2H3
InchiKey:	MCVVUJPXSBQTRZ-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC=CC(=O)OC
Mol. weight [g/mol]:	100.12
CAS:	18707-60-3

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	744.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	755.00		NIST Webbook
ripol	1119.00		NIST Webbook
ripol	1103.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1103.00		NIST Webbook
ripol	1103.00		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

Sources

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=C18707603&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
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