2-Butenoic acid, 1-methylpropyl ester, (E)-

Other names:	Crotonic acid, sec-butyl ester
	sec-Butyl Crotonate
	(E)-2-Butenoic acid 1-methylpropyl ester
Inchi:	InChI=1S/C8H14O2/c1-4-6-8(9)10-7(3)5-2/h4,6-7H,5H2,1-3H3/b6-4+
InchiKey:	KAKJZWSUVDRWQU-GQCTYLIASA-N
Formula:	C8H14O2
SMILES:	CC=CC(=O)OC(C)CC
Mol. weight [g/mol]:	142.20
CAS:	10371-45-6

Physical Properties

Property code	Value	Unit	Source
chl	-4674.40 ± 1.70	kJ/mol	NIST Webbook
gf	-139.66	kJ/mol	Joback Method
hf	-341.31	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	42.13	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	462.45	K	Joback Method
tc	649.84	K	Joback Method
tf	232.00	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.44	J/mol×K	462.45	Joback Method
cpg	319.53	J/mol×K	618.61	Joback Method
cpg	309.31	J/mol×K	587.38	Joback Method
cpg	298.61	J/mol×K	556.15	Joback Method
cpg	287.40	J/mol×K	524.91	Joback Method

cpg	275.69	J/mol×K	493.68	Joback Method
cpg	329.27	J/mol×K	649.84	Joback Method
dvisc	0.0002021	Pa×s	462.45	Joback Method
dvisc	0.0002682	Pa×s	424.04	Joback Method
dvisc	0.0003767	Pa×s	385.63	Joback Method
dvisc	0.0005704	Pa×s	347.23	Joback Method
dvisc	0.0009575	Pa×s	308.82	Joback Method
dvisc	0.0018620	Pa×s	270.41	Joback Method
dvisc	0.0045131	Pa×s	232.00	Joback Method

Sources

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=C10371456&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume