(E)-2-Butenoic acid propyl ester

Other names:	2-Butenoic acid, propyl ester
	Crotonic acid, propyl ester
	Propyl crotonate
	Propyl 2-butenoate
Inchi:	InChI=1S/C7H12O2/c1-3-5-7(8)9-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey:	ZHDCHCTZRODSEN-HWKANZROSA-N
Formula:	C7H12O2
SMILES:	CC=CC(=O)OCCC
Mol. weight [g/mol]:	128.17
CAS:	10352-87-1

Physical Properties

Property code	Value	Unit	Source
chl	-4026.30 ± 2.50	kJ/mol	NIST Webbook
gf	-145.64	kJ/mol	Joback Method
hf	-395.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-443.00 ± 3.00	kJ/mol	NIST Webbook
hfus	16.88	kJ/mol	Joback Method
hvap	48.00	kJ/mol	NIST Webbook
hvap	48.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
tb	440.01	K	Joback Method
tc	625.03	K	Joback Method
tf	235.73	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.68	J/mol×K	440.01	Joback Method
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	253.64	J/mol×K	532.52	Joback Method
cpg	243.76	J/mol×K	501.68	Joback Method
cpg	233.44	J/mol×K	470.85	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0002208	Pa×s	440.01	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0029377	Pa×s	235.73	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=C10352871&Units=SI

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
hfl: Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume