3-Butenoic acid, propyl ester

Other names: Propyl 3-butenoate
Inchi: InChI=1S/C7H12O2/c1-3-5-7(8)9-6-4-2/h3H,1,4-6H2,2H3
InchiKey: JUKZMMDUYUDTMG-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: C=CCC(=O)OCCC
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-138.02	kJ/mol	Joback Method
hf	-307.18	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	39.66	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	864.00		NIST Webbook
tb	432.53	K	Joback Method
tc	612.55	K	Joback Method
tf	239.05	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.85	J/mol×K	432.53	Joback Method
cpg	271.40	J/mol×K	582.54	Joback Method
cpg	262.44	J/mol×K	552.54	Joback Method
cpg	253.12	J/mol×K	522.54	Joback Method
cpg	243.41	J/mol×K	492.54	Joback Method
cpg	233.32	J/mol×K	462.53	Joback Method
cpg	279.98	J/mol×K	612.55	Joback Method

dvisc	0.0002641	Pa×s	432.53	Joback Method
dvisc	0.0003347	Pa×s	400.28	Joback Method
dvisc	0.0004423	Pa×s	368.04	Joback Method
dvisc	0.0006165	Pa×s	335.79	Joback Method
dvisc	0.0009221	Pa×s	303.54	Joback Method
dvisc	0.0015177	Pa×s	271.30	Joback Method
dvisc	0.0028577	Pa×s	239.05	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=R5399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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