3-BUTEN-1-OL, PROPANOATE

Other names:	3-Butenyl propionate
	Propanoic acid, 3-butenyl ester
	3-Butenyl propanoate
Inchi:	InChI=1S/C7H12O2/c1-3-5-6-9-7(8)4-2/h3H,1,4-6H2,2H3
InchiKey:	IVOGAUVYWHQIBD-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CCCOC(=O)CC
Mol. weight [g/mol]:	128.17

Physical Properties

Property code	Value	Unit	Source
af	0.4259		Cheméo Relay (1.0)
gf	-138.02	kJ/mol	Joback Method
hf	-383.40	kJ/mol	Cheméo Relay (1.0)
hfus	15.39	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-1.19		Cheméo Relay (1.0)
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	864.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	855.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1203.00		NIST Webbook
tb	414.81	K	Cheméo Relay (1.0)
tc	598.34	K	Cheméo Relay (1.0)
tf	185.84	K	Cheméo Relay (1.0)
vc	0.411	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.85	J/mol×K	432.53	Joback Method
cpg	233.32	J/mol×K	462.53	Joback Method
cpg	243.41	J/mol×K	492.54	Joback Method
cpg	253.12	J/mol×K	522.54	Joback Method
cpg	262.44	J/mol×K	552.54	Joback Method
cpg	271.40	J/mol×K	582.54	Joback Method
cpg	279.98	J/mol×K	612.55	Joback Method
dvisc	0.0028577	Pa×s	239.05	Joback Method
dvisc	0.0015177	Pa×s	271.30	Joback Method
dvisc	0.0009221	Pa×s	303.54	Joback Method
dvisc	0.0006165	Pa×s	335.79	Joback Method
dvisc	0.0004423	Pa×s	368.04	Joback Method
dvisc	0.0003347	Pa×s	400.28	Joback Method
dvisc	0.0002641	Pa×s	432.53	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27819063&Units=SI

Legend

af: Acentric Factor
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
ie:	Ionization energy
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