Butanoic acid, 1-ethenylhexyl ester

Other names:	Amylvinylcarbinyl butyrate
	1-Octen-3-yl butyrate
	Butyric acid, 1-vinylhexyl ester
	1-Octen-3-ol butyrate
	Butyric acid, 1-pentylallyl ester
	1-Pentylallyl butyrate
	1-Pentyl-2-propenyl butyrate
	Oct-1-en-3-yl butyrate
Inchi:	InChI=1S/C12H22O2/c1-4-7-8-10-11(6-3)14-12(13)9-5-2/h6,11H,3-5,7-10H2,1-2H3
InchiKey:	LZWFXVJBIZIHCH-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	C=CC(CCCCC)OC(=O)CCC
Mol. weight [g/mol]:	198.30
CAS:	16491-54-6

Physical Properties

Property code	Value	Unit	Source
gf	-98.36	kJ/mol	Joback Method
hf	-415.66	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	50.40	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.465		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
tb	546.49	K	Joback Method
tc	722.36	K	Joback Method
tf	280.40	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.62	J/mol×K	546.49	Joback Method

cpg	515.75	J/mol×K	693.05	Joback Method
cpg	502.77	J/mol×K	663.74	Joback Method
cpg	489.19	J/mol×K	634.42	Joback Method
cpg	474.98	J/mol×K	605.11	Joback Method
cpg	460.13	J/mol×K	575.80	Joback Method
cpg	528.12	J/mol×K	722.36	Joback Method
dvisc	0.0001814	Pa×s	546.49	Joback Method
dvisc	0.0002419	Pa×s	502.14	Joback Method
dvisc	0.0003412	Pa×s	457.79	Joback Method
dvisc	0.0005179	Pa×s	413.44	Joback Method
dvisc	0.0008691	Pa×s	369.10	Joback Method
dvisc	0.0016799	Pa×s	324.75	Joback Method
dvisc	0.0039999	Pa×s	280.40	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=C16491546&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume