1,5-Dimethyl-1-vinyl-4-hexenyl butyrate

Other names:	Linalyl butyrate
	Butanoic acid, 1-ethenyl-1,5-dimethyl-4-hexenyl ester
	Butyric acid, linalyl ester
	Butyric acid, 1,5-dimethyl-1-vinyl-4-hexenyl ester
	Linalyl butanoate
Inchi:	InChI=1S/C14H24O2/c1-6-9-13(15)16-14(5,7-2)11-8-10-12(3)4/h7,10H,2,6,8-9,11H2,1,3-
InchiKey:	FHLGUOHLUFIAAA-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	C=CC(C)(CCC=C(C)C)OC(=O)CCC
Mol. weight [g/mol]:	224.34
CAS:	78-36-4

Physical Properties

Property code	Value	Unit	Source
gf	-4.57	kJ/mol	Joback Method
hf	-352.98	kJ/mol	Joback Method
hfus	25.00	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.021		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1408.20		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	593.50	K	Joback Method
tc	781.84	K	Joback Method
tf	301.32	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.80	J/mol×K	593.50	Joback Method
cpg	545.80	J/mol×K	624.89	Joback Method
cpg	561.90	J/mol×K	656.28	Joback Method
cpg	577.14	J/mol×K	687.67	Joback Method
cpg	591.56	J/mol×K	719.06	Joback Method
cpg	605.21	J/mol×K	750.45	Joback Method
cpg	618.13	J/mol×K	781.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78364&Units=SI
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

Legend

cpg: Ideal gas heat capacity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume