Pentanoic acid, 1-ethenyl-1,5-dimethyl-4-hexenyl ester

Other names: Linalyl valerate
Linalyl N-valerate
1,5-dimethyl-1-vinylhex-4-enyl valerate

Inchi: InChI=1S/C15H26O2/c1-6-8-11-14(16)17-15(5,7-2)12-9-10-13(3)4/h7,10H,2,6,8-9,11-12

InchiKey: BYTYEUINJPKZIB-UHFFFAOYSA-N

Formula: C15H26O2

SMILES: C=CC(C)(CCC=C(C)C)OC(=O)CCCC

Mol. weight [g/mol]: 238.37

CAS: 10471-96-2

Physical Properties

Property code	Value	Unit	Source
gf	3.85	kJ/mol	Joback Method
hf	-373.62	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.411		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	616.38	K	Joback Method
tc	802.75	K	Joback Method
tf	312.59	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.05	J/mol×K	616.38	Joback Method
cpg	598.48	J/mol×K	647.44	Joback Method
cpg	615.00	J/mol×K	678.50	Joback Method

cpg	630.65	J/mol×K	709.57	Joback Method
cpg	645.47	J/mol×K	740.63	Joback Method
cpg	659.50	J/mol×K	771.69	Joback Method
cpg	672.80	J/mol×K	802.75	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=C10471962&Units=SI

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