Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester

Other names: Linalyl 3-methylbutanoate
Linalyl iso-valerate
Isovaleric acid, linalyl ester
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexen-1-yl ester
1,6-Octadien-3-ol, 3,7-dimethyl-, isovalerate
1,5-dimethyl-1-vinylhex-4-enyl isovalerate

Inchi: InChI=1S/C15H26O2/c1-7-15(6,10-8-9-12(2)3)17-14(16)11-13(4)5/h7,9,13H,1,8,10-11H2

InchiKey: WCDGWAIZRYMVOW-UHFFFAOYSA-N

Formula: C15H26O2

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

Mol. weight [g/mol]: 238.37

CAS: 1118-27-0

Physical Properties

Property code	Value	Unit	Source
gf	1.41	kJ/mol	Joback Method
hf	-378.90	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.267		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
ripol	1853.00		NIST Webbook
tb	615.94	K	Joback Method
tc	805.63	K	Joback Method
tf	297.59	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.43	J/mol×K	615.94	Joback Method
cpg	599.22	J/mol×K	647.55	Joback Method
cpg	616.05	J/mol×K	679.17	Joback Method
cpg	631.97	J/mol×K	710.78	Joback Method
cpg	647.03	J/mol×K	742.40	Joback Method
cpg	661.27	J/mol×K	774.01	Joback Method
cpg	674.74	J/mol×K	805.63	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1118270&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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