Linalyl isobutyrate

Other names:	1,5-Dimethyl-1-vinyl-4-hexenyl isobutyrate
	Propanoic acid, 2-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester
	Isobutyric acid, 1,5-dimethyl-1-vinyl-4-hexenyl ester
	Linalool isobutyrate
	1,6-Octadien-3-ol, 3,7-dimethyl-, isobutyrate
	3,7-Dimethyl-1,6-octadien-3-yl isobutyrate
	3,7-Dimethyl-1,6-octadienyl isobutyrate
	1,5-Dimethyl-1-vinyl-4-hexenyl 2-methylpropanoate
	Linalyl 2-methylpropanoate
	Isobutyric acid, linalyl ester
	NSC 46145
	Propanoic acid, 2-methyl-, 1-ethenyl-1,5-dimethyl-4-hexen-1-yl ester
	Linalol isobutyrate
	1,5-dimethyl-1-vinylhex-4-enyl isobutyrate
Inchi:	InChI=1S/C14H24O2/c1-7-14(6,10-8-9-11(2)3)16-13(15)12(4)5/h7,9,12H,1,8,10H2,2-6H3
InchiKey:	JZIARAQCPRDGAC-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	C=CC(C)(CCC=C(C)C)OC(=O)C(C)C
Mol. weight [g/mol]:	224.34
CAS:	78-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-7.01	kJ/mol	Joback Method
hf	-358.26	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.877		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1361.70		NIST Webbook

rinpol	1379.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1372.00		NIST Webbook
ripol	1622.00		NIST Webbook
tb	593.06	K	Joback Method
tc	784.94	K	Joback Method
tf	286.32	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.16	J/mol×K	593.06	Joback Method
cpg	546.53	J/mol×K	625.04	Joback Method
cpg	562.95	J/mol×K	657.02	Joback Method
cpg	578.48	J/mol×K	689.00	Joback Method
cpg	593.15	J/mol×K	720.98	Joback Method
cpg	607.02	J/mol×K	752.96	Joback Method
cpg	620.12	J/mol×K	784.94	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=C78353&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

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