

LINALYL 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

Physical Properties

Property code	Value	Unit	Source
hf	-499.83	kJ/mol	Cheméo Relay (1.0)
hfus	25.00	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.62		Cheméo Relay (1.0)
logp	4.021		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
rinpol	1408.20		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1422.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	512.49	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C78364&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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