linalyl 3-methylhexanoate

Inchi: InChI=1S/C17H30O2/c1-7-10-15(5)13-16(18)19-17(6,8-2)12-9-11-14(3)4/h8,11,15H,2,7,9
InchiKey: VCVSHHBNQWDSNK-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: C=CC(C)(CCC=C(C)C)OC(=O)CC(C)CCC
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	18.25	kJ/mol	Joback Method
hf	-420.18	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.047		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	661.70	K	Joback Method
tc	847.90	K	Joback Method
tf	320.13	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.03	J/mol×K	661.70	Joback Method
cpg	708.49	J/mol×K	692.73	Joback Method
cpg	725.98	J/mol×K	723.77	Joback Method
cpg	742.55	J/mol×K	754.80	Joback Method
cpg	758.25	J/mol×K	785.83	Joback Method
cpg	773.12	J/mol×K	816.86	Joback Method
cpg	787.20	J/mol×K	847.90	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=R288192&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume