Linalyl heptanoate

Inchi: InChI=1S/C17H30O2/c1-6-8-9-10-13-16(18)19-17(5,7-2)14-11-12-15(3)4/h7,12H,2,6,8-1
InchiKey: APBQXTVQNYJPRE-UHFFFAOYSA-N
Formula: C17H30O2
SMILES: C=CC(C)(CCC=C(C)C)OC(=O)CCCCCC
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	20.69	kJ/mol	Joback Method
hf	-414.90	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.191		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	1670.00		NIST Webbook
ripol	1930.00		NIST Webbook
tb	662.14	K	Joback Method
tc	845.50	K	Joback Method
tf	335.13	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.61	J/mol×K	662.14	Joback Method
cpg	707.75	J/mol×K	692.70	Joback Method
cpg	724.97	J/mol×K	723.26	Joback Method
cpg	741.30	J/mol×K	753.82	Joback Method
cpg	756.78	J/mol×K	784.38	Joback Method
cpg	771.47	J/mol×K	814.94	Joback Method
cpg	785.41	J/mol×K	845.50	Joback Method

Sources

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=R409988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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