Hexanoic acid, 3,5,5-trimethyl-, 2-methyloct-5-en-4-yl ester

Inchi: InChI=1S/C18H32O2/c1-8-9-10-16(11-14(2)3)20-17(19)12-15(4)13-18(5,6)7/h14-16H,8,1

InchiKey: VHJZYHXXUCMOAN-UHFFFAOYSA-N

Formula: C18H32O2

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

Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	65.08	kJ/mol	Joback Method
hf	-411.94	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	64.51	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.820		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	691.98	K	Joback Method
tc	887.88	K	Joback Method
tf	428.30	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.32	J/mol×K	691.98	Joback Method
cpg	770.05	J/mol×K	724.63	Joback Method
cpg	788.70	J/mol×K	757.28	Joback Method
cpg	806.31	J/mol×K	789.93	Joback Method
cpg	822.92	J/mol×K	822.58	Joback Method
cpg	838.57	J/mol×K	855.23	Joback Method
cpg	853.30	J/mol×K	887.88	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=U406930&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