Hexanoic acid, 3,5,5-trimethyl-, oct-3-en-2-yl ester

Inchi: InChI=1S/C17H32O2/c1-7-8-9-10-11-15(3)19-16(18)12-14(2)13-17(4,5)6/h10-11,14-15H

InchiKey: NSCGWDUQAUOFFR-ZHACJKMWSA-N

Formula: C17H32O2

SMILES: CCCCC=CC(C)OC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-63.48	kJ/mol	Joback Method
hf	-541.10	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.127		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	664.70	K	Joback Method
tc	848.69	K	Joback Method
tf	320.85	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.08	J/mol×K	664.70	Joback Method
cpg	799.88	J/mol×K	818.02	Joback Method
cpg	784.51	J/mol×K	787.36	Joback Method
cpg	768.29	J/mol×K	756.69	Joback Method
cpg	751.17	J/mol×K	726.03	Joback Method
cpg	733.12	J/mol×K	695.36	Joback Method
cpg	814.44	J/mol×K	848.69	Joback Method
dvisc	0.0000685	Pa×s	664.70	Joback Method

dvisc	0.0000987	Pa×s	607.39	Joback Method
dvisc	0.0001535	Pa×s	550.08	Joback Method
dvisc	0.0002644	Pa×s	492.77	Joback Method
dvisc	0.0005254	Pa×s	435.47	Joback Method
dvisc	0.0012858	Pa×s	378.16	Joback Method
dvisc	0.0043326	Pa×s	320.85	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=U406929&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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