Hexanoic acid, 3,5,5-trimethyl-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H32O2/c1-14(2)9-10-17(11-15(3)4)21-18(20)12-16(5)13-19(6,7)8/h15-17H

InchiKey: FLZLQYVTCYHIRW-UHFFFAOYSA-N

Formula: C19H32O2

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

Mol. weight [g/mol]: 292.46

Physical Properties

Property code	Value	Unit	Source
gf	152.79	kJ/mol	Joback Method
hf	-316.94	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	66.15	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.986		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
tb	711.42	K	Joback Method
tc	910.99	K	Joback Method
tf	423.85	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.81	J/mol×K	711.42	Joback Method
cpg	802.51	J/mol×K	744.68	Joback Method
cpg	821.10	J/mol×K	777.94	Joback Method
cpg	838.63	J/mol×K	811.20	Joback Method
cpg	855.14	J/mol×K	844.46	Joback Method
cpg	870.67	J/mol×K	877.73	Joback Method
cpg	885.29	J/mol×K	910.99	Joback Method

Sources

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=U406931&Units=SI
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
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