Hexanoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C17H28O2/c1-6-8-9-11-17(18)19-16(13-12-14(3)4)15(5)10-7-2/h15-16H,3,6-11

InchiKey: SJABPZWVTDJILC-UHFFFAOYSA-N

Formula: C17H28O2

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

Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	135.55	kJ/mol	Joback Method
hf	-261.63	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.494		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	669.33	K	Joback Method
tc	860.81	K	Joback Method
tf	413.89	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.40	J/mol×K	669.33	Joback Method
cpg	685.61	J/mol×K	701.24	Joback Method
cpg	702.92	J/mol×K	733.16	Joback Method
cpg	719.33	J/mol×K	765.07	Joback Method
cpg	734.87	J/mol×K	796.98	Joback Method
cpg	749.57	J/mol×K	828.89	Joback Method
cpg	763.46	J/mol×K	860.81	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=U299358&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