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

Inchi: InChI=1S/C19H32O2/c1-6-8-9-10-11-13-19(20)21-18(15-14-16(3)4)17(5)12-7-2/h17-18H

InchiKey: YTDNGZQHBSSRQN-UHFFFAOYSA-N

Formula: C19H32O2

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

Mol. weight [g/mol]: 292.46

Physical Properties

Property code	Value	Unit	Source
gf	152.39	kJ/mol	Joback Method
hf	-302.91	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.274		Crippen Method
mcvol	273.110	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	1835.00		NIST Webbook
tb	715.09	K	Joback Method
tc	903.91	K	Joback Method
tf	436.43	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.35	J/mol×K	715.09	Joback Method
cpg	799.21	J/mol×K	746.56	Joback Method
cpg	817.10	J/mol×K	778.03	Joback Method
cpg	834.05	J/mol×K	809.50	Joback Method
cpg	850.10	J/mol×K	840.97	Joback Method
cpg	865.26	J/mol×K	872.44	Joback Method
cpg	879.56	J/mol×K	903.91	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=U299347&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume