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

Inchi: InChI=1S/C17H26O2/c1-6-7-8-9-10-17(18)19-16(13-15(4)5)12-11-14(2)3/h9-10,15-16H,2

InchiKey: UATXZPRBFVDGPA-MDZDMXLPSA-N

Formula: C17H26O2

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

Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	215.77	kJ/mol	Joback Method
hf	-144.41	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.270		Crippen Method
mcvol	240.630	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	673.49	K	Joback Method
tc	871.65	K	Joback Method
tf	408.81	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.58	J/mol×K	673.49	Joback Method
cpg	663.37	J/mol×K	706.52	Joback Method
cpg	680.22	J/mol×K	739.54	Joback Method
cpg	696.17	J/mol×K	772.57	Joback Method
cpg	711.25	J/mol×K	805.59	Joback Method
cpg	725.50	J/mol×K	838.62	Joback Method
cpg	738.97	J/mol×K	871.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406944&Units=SI
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

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