Octanoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H30O2/c1-6-7-8-9-10-11-18(19)20-17(14-16(4)5)13-12-15(2)3/h16-17H,2,6

InchiKey: GDLMJDWMTXRVLS-UHFFFAOYSA-N

Formula: C18H30O2

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

Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
gf	143.97	kJ/mol	Joback Method
hf	-282.27	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	65.60	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.884		Crippen Method
mcvol	259.020	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	692.21	K	Joback Method
tc	882.14	K	Joback Method
tf	425.16	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.28	J/mol×K	692.21	Joback Method
cpg	741.84	J/mol×K	723.87	Joback Method
cpg	759.45	J/mol×K	755.52	Joback Method
cpg	776.15	J/mol×K	787.18	Joback Method
cpg	791.96	J/mol×K	818.83	Joback Method
cpg	806.91	J/mol×K	850.49	Joback Method
cpg	821.03	J/mol×K	882.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299346&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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