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

Inchi: InChI=1S/C18H28O2/c1-6-7-8-9-10-11-18(19)20-17(14-16(4)5)13-12-15(2)3/h9-10,16-17

InchiKey: UELHPAAKTOJDNY-MDZDMXLPSA-N

Formula: C18H28O2

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

Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	224.19	kJ/mol	Joback Method
hf	-165.05	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	65.56	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.660		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	696.37	K	Joback Method
tc	892.50	K	Joback Method
tf	420.08	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.89	J/mol×K	696.37	Joback Method
cpg	719.02	J/mol×K	729.06	Joback Method
cpg	736.19	J/mol×K	761.75	Joback Method
cpg	752.44	J/mol×K	794.43	Joback Method
cpg	767.81	J/mol×K	827.12	Joback Method
cpg	782.35	J/mol×K	859.81	Joback Method
cpg	796.08	J/mol×K	892.50	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=U406952&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