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

Inchi: InChI=1S/C15H24O2/c1-11(2)8-9-13(10-12(3)4)17-14(16)15(5,6)7/h12-13H,1,10H2,2-7H

InchiKey: SJZWGKHBXAVXAP-UHFFFAOYSA-N

Formula: C15H24O2

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

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	121.55	kJ/mol	Joback Method
hf	-229.10	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	57.63	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.570		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1360.00		NIST Webbook
tb	620.34	K	Joback Method
tc	826.68	K	Joback Method
tf	393.77	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.38	J/mol×K	620.34	Joback Method
cpg	580.59	J/mol×K	654.73	Joback Method
cpg	597.76	J/mol×K	689.12	Joback Method
cpg	613.95	J/mol×K	723.51	Joback Method
cpg	629.19	J/mol×K	757.90	Joback Method
cpg	643.53	J/mol×K	792.29	Joback Method
cpg	657.01	J/mol×K	826.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299335&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