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

Inchi: InChI=1S/C14H20O4/c1-10(2)6-7-13(8-11(3)4)18-14(16)9-17-12(5)15/h11,13H,1,8-9H2,2

InchiKey: AFGKYZOSXBFLGK-UHFFFAOYSA-N

Formula: C14H20O4

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

Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-123.63	kJ/mol	Joback Method
hf	-444.51	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	65.86	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.087		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	676.98	K	Joback Method
tc	880.47	K	Joback Method
tf	452.24	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.11	J/mol×K	676.98	Joback Method
cpg	571.35	J/mol×K	710.89	Joback Method
cpg	585.75	J/mol×K	744.81	Joback Method
cpg	599.32	J/mol×K	778.72	Joback Method
cpg	612.07	J/mol×K	812.64	Joback Method
cpg	623.99	J/mol×K	846.55	Joback Method
cpg	635.09	J/mol×K	880.47	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=U299207&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