Acetoxyacetic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C13H20O4/c1-5-6-7-12(8-10(2)3)17-13(15)9-16-11(4)14/h10,12H,5,8-9H2,1-4H

InchiKey: NVGYEUSKBYNAND-UHFFFAOYSA-N

Formula: C13H20O4

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

Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-211.34	kJ/mol	Joback Method
hf	-539.51	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.921		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	657.54	K	Joback Method
tc	857.20	K	Joback Method
tf	456.69	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.91	J/mol×K	657.54	Joback Method
cpg	542.01	J/mol×K	690.82	Joback Method
cpg	556.34	J/mol×K	724.09	Joback Method
cpg	569.89	J/mol×K	757.37	Joback Method
cpg	582.66	J/mol×K	790.65	Joback Method
cpg	594.65	J/mol×K	823.92	Joback Method
cpg	605.85	J/mol×K	857.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299206&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