Acetoxyacetic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C9H10O4/c1-3-4-5-6-12-9(11)7-13-8(2)10/h1,4-5H,6-7H2,2H3
InchiKey: LBWYRFGDVNLWTE-UHFFFAOYSA-N
Formula: C9H10O4
SMILES: C#CC=CCOC(=O)COC(C)=O
Mol. weight [g/mol]: 182.17

Physical Properties

Property code	Value	Unit	Source
gf	-139.65	kJ/mol	Joback Method
hf	-309.57	kJ/mol	Joback Method
hfus	27.82	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.282		Crippen Method
mcvol	139.650	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1274.00		NIST Webbook
tb	552.18	K	Joback Method
tc	753.92	K	Joback Method
tf	377.40	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.21	J/mol×K	552.18	Joback Method
cpg	321.63	J/mol×K	585.80	Joback Method
cpg	331.54	J/mol×K	619.43	Joback Method
cpg	340.94	J/mol×K	653.05	Joback Method
cpg	349.85	J/mol×K	686.67	Joback Method
cpg	358.27	J/mol×K	720.29	Joback Method
cpg	366.21	J/mol×K	753.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299204&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