Acetoxyacetic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C10H14O4/c1-4-6-9(5-2)14-10(12)7-13-8(3)11/h9H,5,7H2,1-3H3
InchiKey: SRTYDEDBRGXGAT-UHFFFAOYSA-N
Formula: C10H14O4
SMILES: CC#CC(CC)OC(=O)COC(C)=O
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
gf	-234.16	kJ/mol	Joback Method
hf	-472.31	kJ/mol	Joback Method
hfus	26.83	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.895		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1319.00		NIST Webbook
tb	589.34	K	Joback Method
tc	793.61	K	Joback Method
tf	437.88	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.07	J/mol×K	589.34	Joback Method
cpg	389.79	J/mol×K	623.39	Joback Method
cpg	401.92	J/mol×K	657.43	Joback Method
cpg	413.47	J/mol×K	691.48	Joback Method
cpg	424.43	J/mol×K	725.52	Joback Method
cpg	434.77	J/mol×K	759.57	Joback Method
cpg	444.50	J/mol×K	793.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299205&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

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