Acetoxyacetic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C17H28O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-20-17(19)15-21-16(2)18/h3-11,14
InchiKey: WVTRWCMTBOKAFL-UHFFFAOYSA-N
Formula: C17H28O4
SMILES: CCCCCCCCCCC#CCOC(=O)COC(C)=O
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-172.78	kJ/mol	Joback Method
hf	-611.51	kJ/mol	Joback Method
hfus	48.48	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.627		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	749.94	K	Joback Method
tc	938.40	K	Joback Method
tf	531.77	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.48	J/mol×K	749.94	Joback Method
cpg	760.80	J/mol×K	781.35	Joback Method
cpg	776.24	J/mol×K	812.76	Joback Method
cpg	790.80	J/mol×K	844.17	Joback Method
cpg	804.49	J/mol×K	875.58	Joback Method
cpg	817.31	J/mol×K	906.99	Joback Method
cpg	829.28	J/mol×K	938.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299210&Units=SI

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