Acetoxyacetic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C16H26O4/c1-3-4-5-6-7-8-9-10-11-12-13-19-16(18)14-20-15(2)17/h3,6-14H2,1
InchiKey: JKUZFGVJIGLVNV-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: CCC#CCCCCCCCCOC(=O)COC(C)=O
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-181.20	kJ/mol	Joback Method
hf	-590.87	kJ/mol	Joback Method
hfus	45.89	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.237		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	727.06	K	Joback Method
tc	915.93	K	Joback Method
tf	520.50	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.04	J/mol×K	727.06	Joback Method
cpg	703.99	J/mol×K	758.54	Joback Method
cpg	719.09	J/mol×K	790.02	Joback Method
cpg	733.36	J/mol×K	821.50	Joback Method
cpg	746.80	J/mol×K	852.97	Joback Method
cpg	759.41	J/mol×K	884.45	Joback Method
cpg	771.20	J/mol×K	915.93	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=U308319&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