2,2-Dimethylpropanoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H32O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-17(19)18(2,3)4/h5-13,16H2
InchiKey: TWCYLXORKMQJIN-UHFFFAOYSA-N
Formula: C18H32O2
SMILES: CCCCCCCCCCC#CCOC(=O)C(C)(C)C
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	72.40	kJ/mol	Joback Method
hf	-396.10	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	65.67	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.110		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	693.30	K	Joback Method
tc	880.54	K	Joback Method
tf	473.30	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.99	J/mol×K	693.30	Joback Method
cpg	767.76	J/mol×K	724.51	Joback Method
cpg	785.58	J/mol×K	755.71	Joback Method
cpg	802.47	J/mol×K	786.92	Joback Method
cpg	818.47	J/mol×K	818.13	Joback Method
cpg	833.62	J/mol×K	849.33	Joback Method
cpg	847.94	J/mol×K	880.54	Joback Method

Sources

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=U299338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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