2,2-Dimethylpropanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C11H18O2/c1-6-8-9(7-2)13-10(12)11(3,4)5/h9H,7H2,1-5H3
InchiKey: OHXKMFWHFLPFCX-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CC#CC(CC)OC(=O)C(C)(C)C
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	11.02	kJ/mol	Joback Method
hf	-256.90	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.378		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	532.70	K	Joback Method
tc	739.90	K	Joback Method
tf	379.41	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.97	J/mol×K	532.70	Joback Method
cpg	399.70	J/mol×K	567.23	Joback Method
cpg	414.61	J/mol×K	601.77	Joback Method
cpg	428.71	J/mol×K	636.30	Joback Method
cpg	442.04	J/mol×K	670.83	Joback Method
cpg	454.62	J/mol×K	705.37	Joback Method
cpg	466.47	J/mol×K	739.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299332&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume