Hexanoic acid, 3,5,5-trimethyl-, but-3-yn-2-yl ester

Inchi: InChI=1S/C13H22O2/c1-7-11(3)15-12(14)8-10(2)9-13(4,5)6/h1,10-11H,8-9H2,2-6H3
InchiKey: POBDFKNANDDCHF-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C#CC(C)OC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	45.69	kJ/mol	Joback Method
hf	-283.86	kJ/mol	Joback Method
hfus	20.73	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.014		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
tb	559.14	K	Joback Method
tc	754.50	K	Joback Method
tf	327.82	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.02	J/mol×K	559.14	Joback Method
cpg	495.00	J/mol×K	591.70	Joback Method
cpg	511.08	J/mol×K	624.26	Joback Method
cpg	526.29	J/mol×K	656.82	Joback Method
cpg	540.65	J/mol×K	689.38	Joback Method
cpg	554.22	J/mol×K	721.94	Joback Method
cpg	567.02	J/mol×K	754.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406927&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume