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

Inchi: InChI=1S/C10H16O2/c1-4-6-7-8-10(11)12-9(3)5-2/h2,9H,4,6-8H2,1,3H3
InchiKey: KSURAUYMISABRX-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: C#CC(C)OC(=O)CCCCC
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	20.03	kJ/mol	Joback Method
hf	-207.91	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.132		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	804.00		NIST Webbook
rinpol	804.00		NIST Webbook
tb	494.17	K	Joback Method
tc	681.50	K	Joback Method
tf	306.59	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.87	J/mol×K	494.17	Joback Method
cpg	347.16	J/mol×K	525.39	Joback Method
cpg	359.88	J/mol×K	556.61	Joback Method
cpg	372.04	J/mol×K	587.84	Joback Method
cpg	383.66	J/mol×K	619.06	Joback Method
cpg	394.73	J/mol×K	650.28	Joback Method
cpg	405.29	J/mol×K	681.50	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=U299351&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