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

Inchi: InChI=1S/C9H14O2/c1-4-6-7-9(10)11-8(3)5-2/h2,8H,4,6-7H2,1,3H3
InchiKey: OGADSAZXUBMXDM-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: C#CC(C)OC(=O)CCCC
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	11.61	kJ/mol	Joback Method
hf	-187.27	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.742		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	988.60		NIST Webbook
rinpol	988.60		NIST Webbook
tb	471.29	K	Joback Method
tc	660.70	K	Joback Method
tf	295.32	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.74	J/mol×K	471.29	Joback Method
cpg	303.01	J/mol×K	502.86	Joback Method
cpg	314.76	J/mol×K	534.43	Joback Method
cpg	326.00	J/mol×K	566.00	Joback Method
cpg	336.75	J/mol×K	597.57	Joback Method
cpg	347.00	J/mol×K	629.13	Joback Method
cpg	356.77	J/mol×K	660.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292484&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