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

Inchi: InChI=1S/C11H16O2/c1-4-6-7-8-9-11(12)13-10(3)5-2/h2,8-10H,4,6-7H2,1,3H3/b9-8+
InchiKey: FUEUMTYFGBILID-CMDGGOBGSA-N
Formula: C11H16O2
SMILES: C#CC(C)OC(=O)C=CCCCC
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	108.67	kJ/mol	Joback Method
hf	-111.33	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	48.66	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.298		Crippen Method
mcvol	160.390	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1688.00		NIST Webbook
tb	521.21	K	Joback Method
tc	714.72	K	Joback Method
tf	312.78	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.12	J/mol×K	521.21	Joback Method
cpg	374.90	J/mol×K	553.46	Joback Method
cpg	388.00	J/mol×K	585.71	Joback Method
cpg	400.45	J/mol×K	617.97	Joback Method
cpg	412.27	J/mol×K	650.22	Joback Method
cpg	423.48	J/mol×K	682.47	Joback Method
cpg	434.11	J/mol×K	714.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406940&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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