3-Methyl-2-butenoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C9H12O2/c1-5-8(4)11-9(10)6-7(2)3/h1,6,8H,2-4H3
InchiKey: NDRRMESRUFTJAX-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: C#CC(C)OC(=O)C=C(C)C
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
gf	83.28	kJ/mol	Joback Method
hf	-79.84	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	44.29	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.517		Crippen Method
mcvol	132.210	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	475.33	K	Joback Method
tc	677.68	K	Joback Method
tf	276.28	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.77	J/mol×K	475.33	Joback Method
cpg	285.80	J/mol×K	509.05	Joback Method
cpg	297.22	J/mol×K	542.78	Joback Method
cpg	308.05	J/mol×K	576.50	Joback Method
cpg	318.32	J/mol×K	610.23	Joback Method
cpg	328.03	J/mol×K	643.95	Joback Method
cpg	337.23	J/mol×K	677.68	Joback Method

Sources

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=U299308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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