3-Methyl-2-butenoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C11H16O2/c1-5-7-10(6-2)13-11(12)8-9(3)4/h1,8,10H,6-7H2,2-4H3
InchiKey: YKZJFJKXQAFWBH-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: C#CCC(CC)OC(=O)C=C(C)C
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	100.12	kJ/mol	Joback Method
hf	-121.12	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	48.74	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.298		Crippen Method
mcvol	160.390	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1294.00		NIST Webbook
tb	521.09	K	Joback Method
tc	718.09	K	Joback Method
tf	298.82	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.96	J/mol×K	521.09	Joback Method
cpg	374.96	J/mol×K	553.92	Joback Method
cpg	388.25	J/mol×K	586.76	Joback Method
cpg	400.87	J/mol×K	619.59	Joback Method
cpg	412.83	J/mol×K	652.42	Joback Method
cpg	424.17	J/mol×K	685.26	Joback Method
cpg	434.92	J/mol×K	718.09	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=U299311&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