3-Methyl-2-butenoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H22O2/c1-6-7-8-13(9-11(2)3)16-14(15)10-12(4)5/h10-11,13H,6,9H2,1-5H3

InchiKey: IXSBHDLRHLWLPL-UHFFFAOYSA-N

Formula: C14H22O2

SMILES: CCC#CC(CC(C)C)OC(=O)C=C(C)C

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	102.67	kJ/mol	Joback Method
hf	-207.92	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.324		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	608.17	K	Joback Method
tc	810.63	K	Joback Method
tf	376.76	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.95	J/mol×K	608.17	Joback Method
cpg	525.93	J/mol×K	641.91	Joback Method
cpg	542.04	J/mol×K	675.66	Joback Method
cpg	557.32	J/mol×K	709.40	Joback Method
cpg	571.78	J/mol×K	743.14	Joback Method
cpg	585.47	J/mol×K	776.89	Joback Method
cpg	598.40	J/mol×K	810.63	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=U299313&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume