3-Methyl-2-butenoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C15H22O2/c1-11(2)7-8-14(9-12(3)4)17-15(16)10-13(5)6/h10,12,14H,1,9H2,2-6

InchiKey: YIGBVEXDZVDCJX-UHFFFAOYSA-N

Formula: C15H22O2

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

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	190.38	kJ/mol	Joback Method
hf	-112.92	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	58.96	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.490		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	627.61	K	Joback Method
tc	834.21	K	Joback Method
tf	372.31	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.59	J/mol×K	627.61	Joback Method
cpg	555.77	J/mol×K	662.04	Joback Method
cpg	572.03	J/mol×K	696.48	Joback Method
cpg	587.40	J/mol×K	730.91	Joback Method
cpg	601.92	J/mol×K	765.34	Joback Method
cpg	615.62	J/mol×K	799.78	Joback Method
cpg	628.55	J/mol×K	834.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299314&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