2,2-Dimethylpropanoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H24O2/c1-7-8-9-12(10-11(2)3)16-13(15)14(4,5)6/h11-12H,7,10H2,1-6H3

InchiKey: CPFVDMGMVWCYGU-UHFFFAOYSA-N

Formula: C14H24O2

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

Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	33.84	kJ/mol	Joback Method
hf	-324.10	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.404		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
tb	600.90	K	Joback Method
tc	803.06	K	Joback Method
tf	398.22	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.20	J/mol×K	600.90	Joback Method
cpg	550.22	J/mol×K	634.59	Joback Method
cpg	567.28	J/mol×K	668.29	Joback Method
cpg	583.40	J/mol×K	701.98	Joback Method
cpg	598.63	J/mol×K	735.67	Joback Method
cpg	612.98	J/mol×K	769.36	Joback Method
cpg	626.51	J/mol×K	803.06	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=U299334&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