Cyclopropanecarboxylic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C14H20O2/c1-10(2)5-8-13(9-11(3)4)16-14(15)12-6-7-12/h11-13H,1,6-7,9H2,2-

InchiKey: YZKCWJQTDUOUNL-UHFFFAOYSA-N

Formula: C14H20O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)C1CC1

Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	171.04	kJ/mol	Joback Method
hf	-126.91	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.934		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1444.00		NIST Webbook
tb	607.43	K	Joback Method
tc	819.24	K	Joback Method
tf	398.02	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.61	J/mol×K	607.43	Joback Method
cpg	511.12	J/mol×K	642.73	Joback Method
cpg	527.63	J/mol×K	678.03	Joback Method
cpg	543.17	J/mol×K	713.33	Joback Method
cpg	557.80	J/mol×K	748.64	Joback Method
cpg	571.57	J/mol×K	783.94	Joback Method
cpg	584.53	J/mol×K	819.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299379&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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