2,2-Dimethylpropanoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C16H26O2/c1-8-9-13(4)14(11-10-12(2)3)18-15(17)16(5,6)7/h13-14H,2,8-9H2,1

InchiKey: DDZBSMWOQSKQFI-UHFFFAOYSA-N

Formula: C16H26O2

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

Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	129.97	kJ/mol	Joback Method
hf	-249.74	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.960		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	643.22	K	Joback Method
tc	846.59	K	Joback Method
tf	405.04	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.47	J/mol×K	643.22	Joback Method
cpg	634.05	J/mol×K	677.11	Joback Method
cpg	651.59	J/mol×K	711.01	Joback Method
cpg	668.12	J/mol×K	744.90	Joback Method
cpg	683.71	J/mol×K	778.80	Joback Method
cpg	698.38	J/mol×K	812.69	Joback Method
cpg	712.18	J/mol×K	846.59	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=U299336&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