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

Inchi: InChI=1S/C15H22O4/c1-6-7-12(4)14(9-8-11(2)3)19-15(17)10-18-13(5)16/h12,14H,2,6-7,

InchiKey: PEFAJKNLWUCYSW-UHFFFAOYSA-N

Formula: C15H22O4

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

Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-115.21	kJ/mol	Joback Method
hf	-465.15	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.477		Crippen Method
mcvol	224.190	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	699.86	K	Joback Method
tc	900.95	K	Joback Method
tf	463.51	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.50	J/mol×K	699.86	Joback Method
cpg	625.19	J/mol×K	733.37	Joback Method
cpg	640.00	J/mol×K	766.89	Joback Method
cpg	653.94	J/mol×K	800.40	Joback Method
cpg	667.02	J/mol×K	833.92	Joback Method
cpg	679.25	J/mol×K	867.43	Joback Method
cpg	690.63	J/mol×K	900.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299208&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