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

Inchi: InChI=1S/C16H24O2/c1-7-8-14(6)15(10-9-12(2)3)18-16(17)11-13(4)5/h11,14-15H,2,7-8H
InchiKey: IMLTUEABADLIIT-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: C=C(C)C#CC(OC(=O)C=C(C)C)C(C)CCC
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	198.80	kJ/mol	Joback Method
hf	-133.56	kJ/mol	Joback Method
hfus	32.36	kJ/mol	Joback Method
hvap	61.19	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.880		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
tb	650.49	K	Joback Method
tc	854.13	K	Joback Method
tf	383.58	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.26	J/mol×K	650.49	Joback Method
cpg	608.89	J/mol×K	684.43	Joback Method
cpg	625.58	J/mol×K	718.37	Joback Method
cpg	641.36	J/mol×K	752.31	Joback Method
cpg	656.28	J/mol×K	786.25	Joback Method
cpg	670.36	J/mol×K	820.19	Joback Method
cpg	683.64	J/mol×K	854.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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