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

Inchi: InChI=1S/C16H26O2/c1-6-7-8-9-16(17)18-15(12-14(4)5)11-10-13(2)3/h14-15H,2,6-9,12H
InchiKey: DBEQUMZHKFWGOD-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CCCCC
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	127.13	kJ/mol	Joback Method
hf	-240.99	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.104		Crippen Method
mcvol	230.840	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	646.45	K	Joback Method
tc	839.85	K	Joback Method
tf	402.62	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.78	J/mol×K	646.45	Joback Method
cpg	630.61	J/mol×K	678.68	Joback Method
cpg	647.55	J/mol×K	710.92	Joback Method
cpg	663.62	J/mol×K	743.15	Joback Method
cpg	678.85	J/mol×K	775.39	Joback Method
cpg	693.26	J/mol×K	807.62	Joback Method
cpg	706.88	J/mol×K	839.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299357&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

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