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

Inchi: InChI=1S/C15H24O2/c1-6-7-8-15(16)17-14(11-13(4)5)10-9-12(2)3/h13-14H,2,6-8,11H2,1

InchiKey: KJQMUNADTYHASA-UHFFFAOYSA-N

Formula: C15H24O2

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

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	118.71	kJ/mol	Joback Method
hf	-220.35	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	58.93	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.714		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
tb	623.57	K	Joback Method
tc	819.24	K	Joback Method
tf	391.35	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.51	J/mol×K	623.57	Joback Method
cpg	576.89	J/mol×K	656.18	Joback Method
cpg	593.41	J/mol×K	688.79	Joback Method
cpg	609.09	J/mol×K	721.40	Joback Method
cpg	623.95	J/mol×K	754.02	Joback Method
cpg	638.02	J/mol×K	786.63	Joback Method
cpg	651.31	J/mol×K	819.24	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=U292489&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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