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

Inchi: InChI=1S/C14H22O2/c1-6-7-14(15)16-13(10-12(4)5)9-8-11(2)3/h12-13H,2,6-7,10H2,1,3-

InchiKey: LEJKEOGIMLHRRZ-UHFFFAOYSA-N

Formula: C14H22O2

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

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	110.29	kJ/mol	Joback Method
hf	-199.71	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.324		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
tb	600.69	K	Joback Method
tc	798.91	K	Joback Method
tf	380.08	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.69	J/mol×K	600.69	Joback Method
cpg	524.54	J/mol×K	633.73	Joback Method
cpg	540.57	J/mol×K	666.76	Joback Method
cpg	555.78	J/mol×K	699.80	Joback Method
cpg	570.21	J/mol×K	732.84	Joback Method
cpg	583.87	J/mol×K	765.88	Joback Method
cpg	596.78	J/mol×K	798.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299123&Units=SI

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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