Valeric acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H24O2/c1-5-7-9-13(11-12(3)4)16-14(15)10-8-6-2/h12-13H,5-6,8,10-11H2,1
InchiKey: JOVMXOXEEIDZSS-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: CCC#CC(CC(C)C)OC(=O)CCCC
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	31.00	kJ/mol	Joback Method
hf	-315.35	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.548		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1455.30		NIST Webbook
rinpol	1455.30		NIST Webbook
tb	604.13	K	Joback Method
tc	795.74	K	Joback Method
tf	395.80	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.27	J/mol×K	604.13	Joback Method
cpg	546.42	J/mol×K	636.06	Joback Method
cpg	562.78	J/mol×K	668.00	Joback Method
cpg	578.36	J/mol×K	699.93	Joback Method
cpg	593.16	J/mol×K	731.87	Joback Method
cpg	607.22	J/mol×K	763.80	Joback Method
cpg	620.53	J/mol×K	795.74	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=U292488&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