Octanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H24O2/c1-4-7-8-9-10-12-14(15)16-13(6-3)11-5-2/h13H,4,6-10,12H2,1-3H3
InchiKey: UIYXGURQBFLUSB-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: CC#CC(CC)OC(=O)CCCCCCC
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	33.44	kJ/mol	Joback Method
hf	-310.07	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	57.68	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.692		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	604.57	K	Joback Method
tc	792.72	K	Joback Method
tf	410.80	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.90	J/mol×K	604.57	Joback Method
cpg	545.69	J/mol×K	635.93	Joback Method
cpg	561.73	J/mol×K	667.29	Joback Method
cpg	577.02	J/mol×K	698.64	Joback Method
cpg	591.58	J/mol×K	730.00	Joback Method
cpg	605.42	J/mol×K	761.36	Joback Method
cpg	618.55	J/mol×K	792.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299343&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