Octanoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H20O2/c1-3-5-7-8-9-11-13(14)15-12-10-6-4-2/h2,6,10H,3,5,7-9,11-12H2,1
InchiKey: QSUKOVORNGWCOD-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: C#CC=CCOC(=O)CCCCCCC
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	127.95	kJ/mol	Joback Method
hf	-147.33	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.080		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	567.41	K	Joback Method
tc	752.63	K	Joback Method
tf	350.32	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.40	J/mol×K	567.41	Joback Method
cpg	470.33	J/mol×K	598.28	Joback Method
cpg	484.55	J/mol×K	629.15	Joback Method
cpg	498.08	J/mol×K	660.02	Joback Method
cpg	510.96	J/mol×K	690.89	Joback Method
cpg	523.20	J/mol×K	721.76	Joback Method
cpg	534.84	J/mol×K	752.63	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=U299342&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume