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

Inchi: InChI=1S/C11H16O2/c1-3-5-7-9-11(12)13-10-8-6-4-2/h2,6,8H,3,5,7,9-10H2,1H3
InchiKey: AIHFDXYXTHADDO-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: C#CC=CCOC(=O)CCCCC
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	111.11	kJ/mol	Joback Method
hf	-106.05	kJ/mol	Joback Method
hfus	30.21	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.299		Crippen Method
mcvol	160.390	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1304.00		NIST Webbook
tb	521.65	K	Joback Method
tc	711.16	K	Joback Method
tf	327.78	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.84	J/mol×K	521.65	Joback Method
cpg	374.28	J/mol×K	553.24	Joback Method
cpg	387.06	J/mol×K	584.82	Joback Method
cpg	399.23	J/mol×K	616.41	Joback Method
cpg	410.80	J/mol×K	647.99	Joback Method
cpg	421.79	J/mol×K	679.58	Joback Method
cpg	432.24	J/mol×K	711.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299353&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

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