Valeric acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H32O2/c1-3-5-7-8-9-10-11-12-13-14-15-17-20-18(19)16-6-4-2/h3-13,16-17
InchiKey: ZQZHZXGGYFSZHR-UHFFFAOYSA-N
Formula: C18H32O2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	69.56	kJ/mol	Joback Method
hf	-387.35	kJ/mol	Joback Method
hfus	48.28	kJ/mol	Joback Method
hvap	66.97	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.254		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	2010.70		NIST Webbook
rinpol	2010.70		NIST Webbook
tb	696.53	K	Joback Method
tc	876.84	K	Joback Method
tf	470.88	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.85	J/mol×K	696.53	Joback Method
cpg	765.14	J/mol×K	726.58	Joback Method
cpg	782.56	J/mol×K	756.63	Joback Method
cpg	799.14	J/mol×K	786.68	Joback Method
cpg	814.90	J/mol×K	816.73	Joback Method
cpg	829.86	J/mol×K	846.79	Joback Method
cpg	844.04	J/mol×K	876.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292492&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