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

Inchi: InChI=1S/C11H18O2/c1-4-7-9-11(12)13-10(6-3)8-5-2/h10H,4,6-7,9H2,1-3H3
InchiKey: JMTGAGXMQUQBSQ-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CC#CC(CC)OC(=O)CCCC
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	8.18	kJ/mol	Joback Method
hf	-248.15	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.522		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1277.60		NIST Webbook
rinpol	1277.60		NIST Webbook
tb	535.93	K	Joback Method
tc	731.09	K	Joback Method
tf	376.99	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.79	J/mol×K	535.93	Joback Method
cpg	395.49	J/mol×K	568.46	Joback Method
cpg	409.57	J/mol×K	600.98	Joback Method
cpg	423.02	J/mol×K	633.51	Joback Method
cpg	435.86	J/mol×K	666.04	Joback Method
cpg	448.09	J/mol×K	698.57	Joback Method
cpg	459.72	J/mol×K	731.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292487&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