Carbonic acid, but-2-yn-1-yl undecyl ester

Inchi: InChI=1S/C16H28O3/c1-3-5-7-8-9-10-11-12-13-15-19-16(17)18-14-6-4-2/h3,5,7-15H2,1-
InchiKey: OPSWHJLDLSKMQZ-UHFFFAOYSA-N
Formula: C16H28O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 268.39

Physical Properties

Property code	Value	Unit	Source
gf	-52.28	kJ/mol	Joback Method
hf	-478.29	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.694		Crippen Method
mcvol	241.010	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	673.19	K	Joback Method
tc	854.70	K	Joback Method
tf	470.57	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.55	J/mol×K	673.19	Joback Method
cpg	681.75	J/mol×K	703.44	Joback Method
cpg	698.16	J/mol×K	733.69	Joback Method
cpg	713.79	J/mol×K	763.94	Joback Method
cpg	728.65	J/mol×K	794.20	Joback Method
cpg	742.74	J/mol×K	824.45	Joback Method
cpg	756.07	J/mol×K	854.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383206&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