Carbonic acid, but-3-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/h2H,3,5-15H2,1

InchiKey: LDLYPXIKWJSBHT-UHFFFAOYSA-N

Formula: C16H28O3

SMILES: C#CCCOC(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 268.39

Physical Properties

Property code	Value	Unit	Source
gf	-32.01	kJ/mol	Joback Method
hf	-458.69	kJ/mol	Joback Method
hfus	44.15	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.694		Crippen Method
mcvol	241.010	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	654.31	K	Joback Method
tc	828.78	K	Joback Method
tf	411.44	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.53	J/mol×K	654.31	Joback Method
cpg	676.29	J/mol×K	683.39	Joback Method
cpg	692.31	J/mol×K	712.47	Joback Method
cpg	707.59	J/mol×K	741.55	Joback Method
cpg	722.16	J/mol×K	770.63	Joback Method
cpg	736.01	J/mol×K	799.70	Joback Method
cpg	749.17	J/mol×K	828.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383177&Units=SI

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