Carbonic acid, but-3-yn-1-yl tetradecyl ester

Inchi: InChI=1S/C19H34O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-19(20)21-17-6-4-2/h2H,3
InchiKey: AKOFDARZRGPJKH-UHFFFAOYSA-N
Formula: C19H34O3
SMILES: C#CCCOC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.47

Physical Properties

Property code	Value	Unit	Source
gf	-6.75	kJ/mol	Joback Method
hf	-520.61	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	69.31	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.864		Crippen Method
mcvol	283.280	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	722.95	K	Joback Method
tc	898.06	K	Joback Method
tf	445.25	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.41	J/mol×K	722.95	Joback Method
cpg	847.48	J/mol×K	752.14	Joback Method
cpg	864.68	J/mol×K	781.32	Joback Method
cpg	881.05	J/mol×K	810.51	Joback Method
cpg	896.58	J/mol×K	839.69	Joback Method
cpg	911.30	J/mol×K	868.88	Joback Method
cpg	925.23	J/mol×K	898.06	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=U383180&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