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

Inchi: InChI=1S/C20H36O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-23-20(21)22-18-6-4-2/h2
InchiKey: WITDLWSORRHZDB-UHFFFAOYSA-N
Formula: C20H36O3
SMILES: C#CCCOC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 324.50

Physical Properties

Property code	Value	Unit	Source
gf	1.67	kJ/mol	Joback Method
hf	-541.25	kJ/mol	Joback Method
hfus	54.51	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.254		Crippen Method
mcvol	297.370	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook
tb	745.83	K	Joback Method
tc	922.19	K	Joback Method
tf	456.52	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.27	J/mol×K	745.83	Joback Method
cpg	906.75	J/mol×K	775.22	Joback Method
cpg	924.32	J/mol×K	804.62	Joback Method
cpg	941.01	J/mol×K	834.01	Joback Method
cpg	956.82	J/mol×K	863.40	Joback Method
cpg	971.79	J/mol×K	892.80	Joback Method
cpg	985.93	J/mol×K	922.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383181&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