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

Inchi: InChI=1S/C23H42O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-26-23(24)25-2
InchiKey: GBLKDTMJEXEGIJ-UHFFFAOYSA-N
Formula: C23H42O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.58

Physical Properties

Property code	Value	Unit	Source
gf	6.66	kJ/mol	Joback Method
hf	-622.77	kJ/mol	Joback Method
hfus	62.42	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.424		Crippen Method
mcvol	339.640	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	833.35	K	Joback Method
tc	1022.11	K	Joback Method
tf	549.46	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.31	J/mol×K	833.35	Joback Method
cpg	1098.17	J/mol×K	864.81	Joback Method
cpg	1116.89	J/mol×K	896.27	Joback Method
cpg	1134.49	J/mol×K	927.73	Joback Method
cpg	1151.00	J/mol×K	959.19	Joback Method
cpg	1166.43	J/mol×K	990.65	Joback Method
cpg	1180.82	J/mol×K	1022.11	Joback Method

Sources

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=U383213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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