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

Inchi: InChI=1S/C22H40O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-25-22(23)24-20-6
InchiKey: FQINAGFWKLGLJC-UHFFFAOYSA-N
Formula: C22H40O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 352.55

Physical Properties

Property code	Value	Unit	Source
gf	-1.76	kJ/mol	Joback Method
hf	-602.13	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.034		Crippen Method
mcvol	325.550	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	810.47	K	Joback Method
tc	996.26	K	Joback Method
tf	538.19	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.45	J/mol×K	810.47	Joback Method
cpg	1035.92	J/mol×K	841.44	Joback Method
cpg	1054.32	J/mol×K	872.40	Joback Method
cpg	1071.66	J/mol×K	903.37	Joback Method
cpg	1087.97	J/mol×K	934.33	Joback Method
cpg	1103.27	J/mol×K	965.30	Joback Method
cpg	1117.57	J/mol×K	996.26	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=U383212&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