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

Inchi: InChI=1S/C21H38O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-21(22)23-19-6-4-2
InchiKey: YSJNPWQADLAFJI-UHFFFAOYSA-N
Formula: C21H38O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 338.52

Physical Properties

Property code	Value	Unit	Source
gf	-10.18	kJ/mol	Joback Method
hf	-581.49	kJ/mol	Joback Method
hfus	57.24	kJ/mol	Joback Method
hvap	76.06	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.644		Crippen Method
mcvol	311.460	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	787.59	K	Joback Method
tc	971.15	K	Joback Method
tf	526.92	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.38	J/mol×K	787.59	Joback Method
cpg	974.48	J/mol×K	818.18	Joback Method
cpg	992.57	J/mol×K	848.78	Joback Method
cpg	1009.66	J/mol×K	879.37	Joback Method
cpg	1025.77	J/mol×K	909.97	Joback Method
cpg	1040.91	J/mol×K	940.56	Joback Method
cpg	1055.10	J/mol×K	971.15	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=U383211&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