Carbonic acid, but-3-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: RQJRBMVHQIOHGG-UHFFFAOYSA-N
Formula: C23H42O3
SMILES: C#CCCOC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.58

Physical Properties

Property code	Value	Unit	Source
gf	26.93	kJ/mol	Joback Method
hf	-603.17	kJ/mol	Joback Method
hfus	62.28	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.424		Crippen Method
mcvol	339.640	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	2529.00		NIST Webbook
rinpol	2529.00		NIST Webbook
tb	814.47	K	Joback Method
tc	998.47	K	Joback Method
tf	490.33	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.44	J/mol×K	814.47	Joback Method
cpg	1090.22	J/mol×K	845.14	Joback Method
cpg	1108.92	J/mol×K	875.80	Joback Method
cpg	1126.58	J/mol×K	906.47	Joback Method
cpg	1143.22	J/mol×K	937.14	Joback Method
cpg	1158.86	J/mol×K	967.80	Joback Method
cpg	1173.55	J/mol×K	998.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383184&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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