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

Inchi: InChI=1S/C19H34O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-19(20)21-17-6-4-2/h3,5,
InchiKey: YDESNQMXTHNGAK-UHFFFAOYSA-N
Formula: C19H34O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.47

Physical Properties

Property code	Value	Unit	Source
gf	-27.02	kJ/mol	Joback Method
hf	-540.21	kJ/mol	Joback Method
hfus	52.06	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.864		Crippen Method
mcvol	283.280	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	741.83	K	Joback Method
tc	922.92	K	Joback Method
tf	504.38	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.90	J/mol×K	741.83	Joback Method
cpg	854.28	J/mol×K	772.01	Joback Method
cpg	871.75	J/mol×K	802.19	Joback Method
cpg	888.32	J/mol×K	832.37	Joback Method
cpg	903.99	J/mol×K	862.56	Joback Method
cpg	918.79	J/mol×K	892.74	Joback Method
cpg	932.72	J/mol×K	922.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383209&Units=SI

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

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