Carbonic acid, but-3-yn-1-yl dodecyl ester

Inchi: InChI=1S/C17H30O3/c1-3-5-7-8-9-10-11-12-13-14-16-20-17(18)19-15-6-4-2/h2H,3,5-16H
InchiKey: MSOFUMVSPAGSSO-UHFFFAOYSA-N
Formula: C17H30O3
SMILES: C#CCCOC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 282.42

Physical Properties

Property code	Value	Unit	Source
gf	-23.59	kJ/mol	Joback Method
hf	-479.33	kJ/mol	Joback Method
hfus	46.74	kJ/mol	Joback Method
hvap	64.86	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.084		Crippen Method
mcvol	255.100	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
tb	677.19	K	Joback Method
tc	851.41	K	Joback Method
tf	422.71	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.95	J/mol×K	677.19	Joback Method
cpg	732.17	J/mol×K	706.23	Joback Method
cpg	748.61	J/mol×K	735.26	Joback Method
cpg	764.28	J/mol×K	764.30	Joback Method
cpg	779.20	J/mol×K	793.34	Joback Method
cpg	793.37	J/mol×K	822.37	Joback Method
cpg	806.82	J/mol×K	851.41	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=U383178&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